



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:15 PM UTC

PDB ID : 4G7Z / pdb_00004g7z
Title : Crystal structure of Thermus thermophilus transcription initiation complex containing 5-BrU at template-strand position +1
Authors : Zhang, Y.; Ebright, R.H.
Deposited on : 2012-07-20
Resolution : 3.81 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

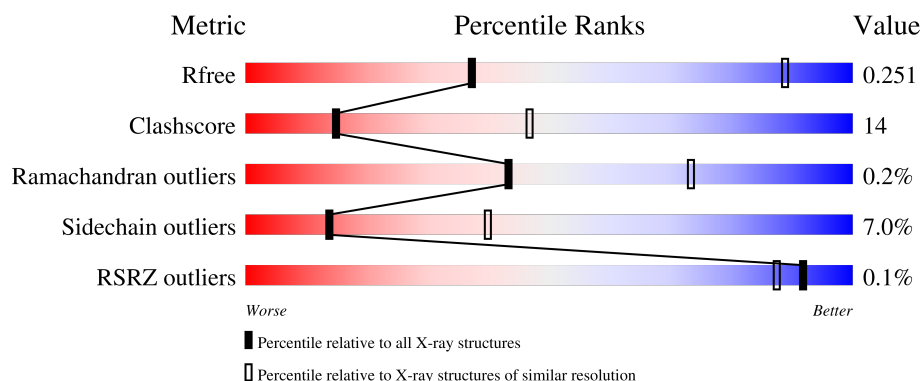
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.81 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}	180053	1043 (3.98-3.66)
Clashscore	190562	1075 (3.98-3.66)
Ramachandran outliers	187476	1029 (3.98-3.66)
Sidechain outliers	187428	1024 (3.98-3.66)
RSRZ outliers	180081	1042 (3.98-3.66)

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

Mol	Chain	Length	Quality of chain
1	A	315	40% 27% 5% 28%
1	B	315	41% 26% • 30%
1	K	315	54% 16% • 28%
1	L	315	52% 18% • 29%
2	C	1119	57% 36% 6% •

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Mol	Chain	Length	Quality of chain
2	M	1119	
3	D	1524	
3	N	1524	
4	E	99	
4	O	99	
5	F	443	
5	P	443	
6	H	27	
6	R	27	
7	G	21	
7	Q	21	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	BRU	Q	15	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 56872 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 DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	226	Total	C	N	O	S	0	0	0
			1782	1138	310	332	2			
1	B	222	Total	C	N	O	S	0	0	0
			1750	1118	304	326	2			
1	K	226	Total	C	N	O	S	0	0	0
			1782	1138	310	332	2			
1	L	225	Total	C	N	O	S	0	0	0
			1773	1133	308	330	2			

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1111	Total	C	N	O	S	0	0	0
			8770	5548	1564	1634	24			
2	M	1111	Total	C	N	O	S	0	0	0
			8770	5548	1564	1634	24			

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1482	Total	C	N	O	S	0	0	0
			11704	7421	2059	2189	35			
3	N	1489	Total	C	N	O	S	0	0	0
			11746	7446	2066	2198	36			

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	94	Total	C	N	O	S	0	0	0
			761	486	132	139	4			
4	O	94	Total	C	N	O	S	0	0	0
			761	486	132	139	4			

- Molecule 5 is a protein called RNA polymerase sigma factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	346	Total	C	N	O	S	0	0	0
			2807	1770	509	524	4			
5	P	347	Total	C	N	O	S	0	0	0
			2814	1774	510	526	4			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-19	MET	-	expression tag	UNP Q5SKW1
F	-18	GLY	-	expression tag	UNP Q5SKW1
F	-17	SER	-	expression tag	UNP Q5SKW1
F	-16	SER	-	expression tag	UNP Q5SKW1
F	-15	HIS	-	expression tag	UNP Q5SKW1
F	-14	HIS	-	expression tag	UNP Q5SKW1
F	-13	HIS	-	expression tag	UNP Q5SKW1
F	-12	HIS	-	expression tag	UNP Q5SKW1
F	-11	HIS	-	expression tag	UNP Q5SKW1
F	-10	HIS	-	expression tag	UNP Q5SKW1
F	-9	SER	-	expression tag	UNP Q5SKW1
F	-8	SER	-	expression tag	UNP Q5SKW1
F	-7	GLY	-	expression tag	UNP Q5SKW1
F	-6	LEU	-	expression tag	UNP Q5SKW1
F	-5	VAL	-	expression tag	UNP Q5SKW1
F	-4	PRO	-	expression tag	UNP Q5SKW1
F	-3	ARG	-	expression tag	UNP Q5SKW1
F	-2	GLY	-	expression tag	UNP Q5SKW1
F	-1	SER	-	expression tag	UNP Q5SKW1
F	0	HIS	-	expression tag	UNP Q5SKW1
P	-19	MET	-	expression tag	UNP Q5SKW1
P	-18	GLY	-	expression tag	UNP Q5SKW1
P	-17	SER	-	expression tag	UNP Q5SKW1
P	-16	SER	-	expression tag	UNP Q5SKW1
P	-15	HIS	-	expression tag	UNP Q5SKW1
P	-14	HIS	-	expression tag	UNP Q5SKW1
P	-13	HIS	-	expression tag	UNP Q5SKW1
P	-12	HIS	-	expression tag	UNP Q5SKW1
P	-11	HIS	-	expression tag	UNP Q5SKW1
P	-10	HIS	-	expression tag	UNP Q5SKW1
P	-9	SER	-	expression tag	UNP Q5SKW1
P	-8	SER	-	expression tag	UNP Q5SKW1
P	-7	GLY	-	expression tag	UNP Q5SKW1
P	-6	LEU	-	expression tag	UNP Q5SKW1

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Chain	Residue	Modelled	Actual	Comment	Reference
P	-5	VAL	-	expression tag	UNP Q5SKW1
P	-4	PRO	-	expression tag	UNP Q5SKW1
P	-3	ARG	-	expression tag	UNP Q5SKW1
P	-2	GLY	-	expression tag	UNP Q5SKW1
P	-1	SER	-	expression tag	UNP Q5SKW1
P	0	HIS	-	expression tag	UNP Q5SKW1

- Molecule 6 is a DNA chain called 5'-D(*TP*AP*TP*AP*AP*TP*GP*GP*GP*AP*GP*C
P*TP*GP*TP*CP*AP*CP*GP*GP*AP*TP*GP*CP*AP*GP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	H	24	Total	C	N	O	P	0	0	0
			495	236	94	142	23			
6	R	24	Total	C	N	O	P	0	0	0
			495	236	94	142	23			

- Molecule 7 is a DNA chain called 5'-D(*CP*CP*TP*GP*CP*AP*TP*CP*CP*GP*TP*G
P*AP*GP*(BRU)P*CP*GP*AP*GP*GP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	16	Total	Br	C	N	O	P	0	0
			328	1	155	63	94	15		
7	Q	16	Total	Br	C	N	O	P	0	0
			328	1	155	63	94	15		

- Molecule 8 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	D	2	Total	Zn	0	0
			2	2		
8	N	2	Total	Zn	0	0
			2	2		

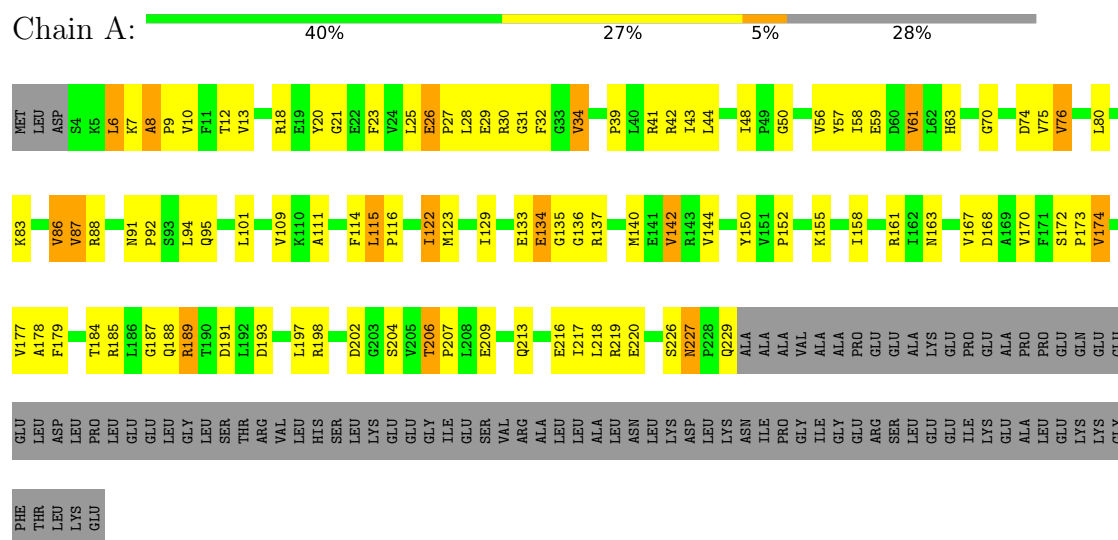
- Molecule 9 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	D	1	Total	Mg	0	0
			1	1		
9	N	1	Total	Mg	0	0
			1	1		

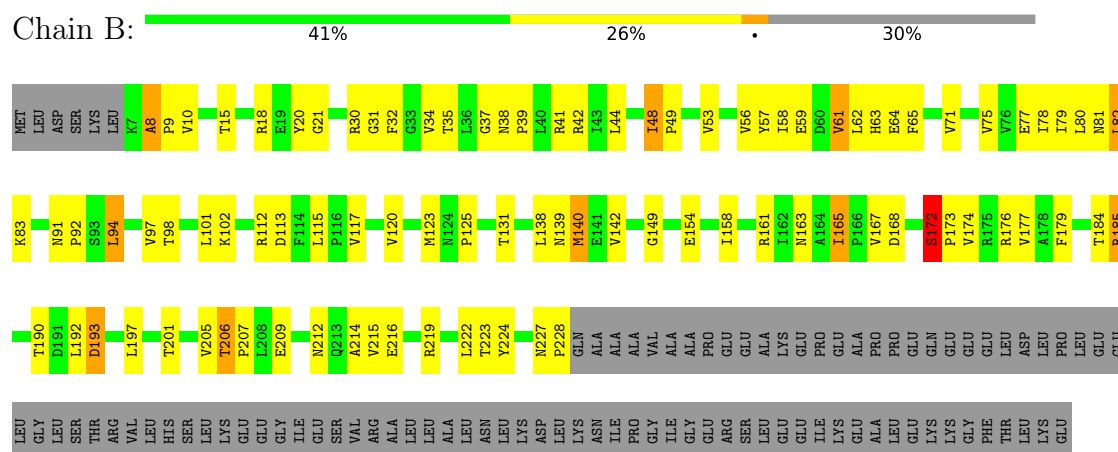
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: DNA-directed RNA polymerase subunit alpha

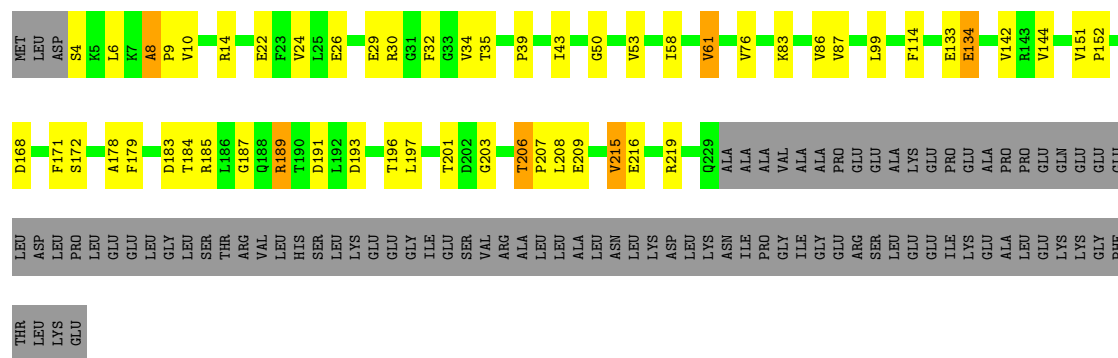


• Molecule 1: DNA-directed RNA polymerase subunit alpha

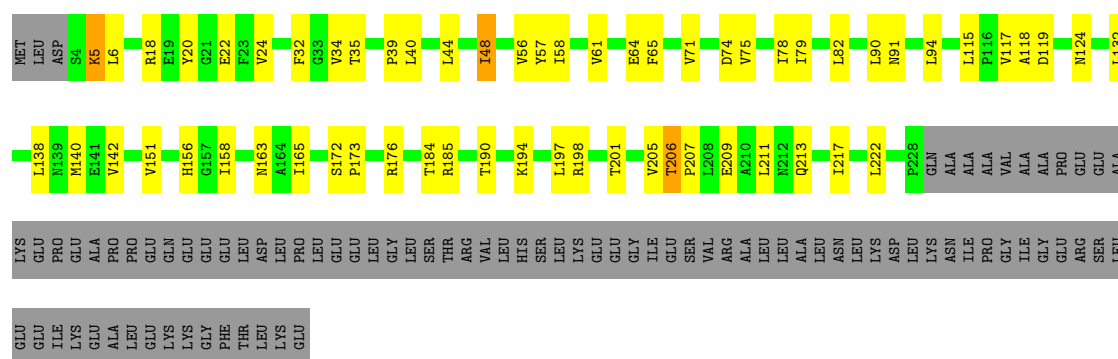


• Molecule 1: DNA-directed RNA polymerase subunit alpha

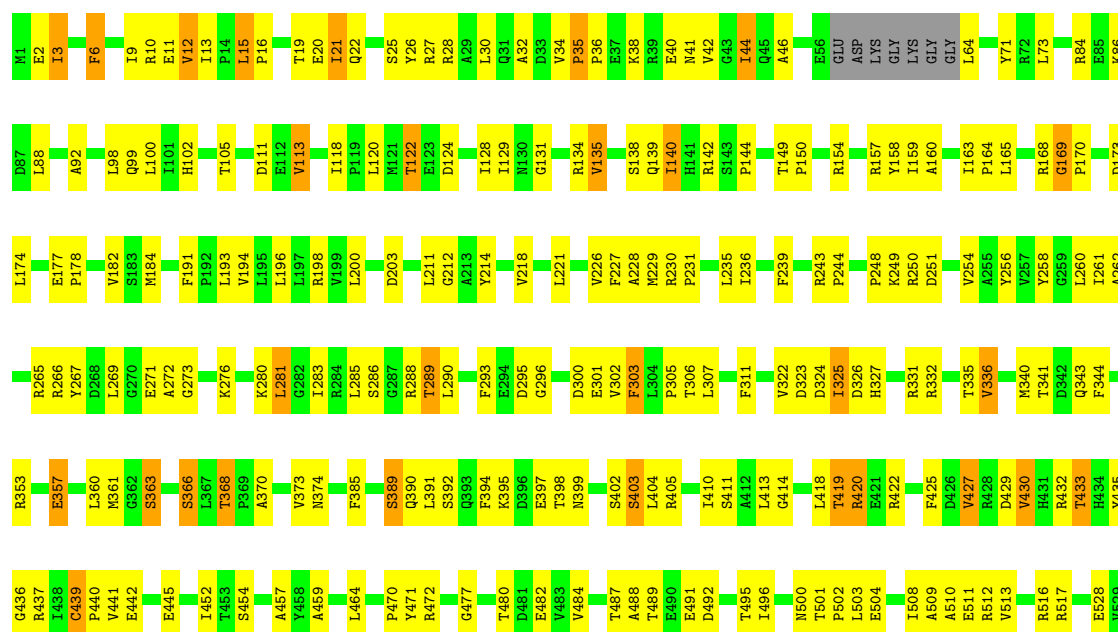


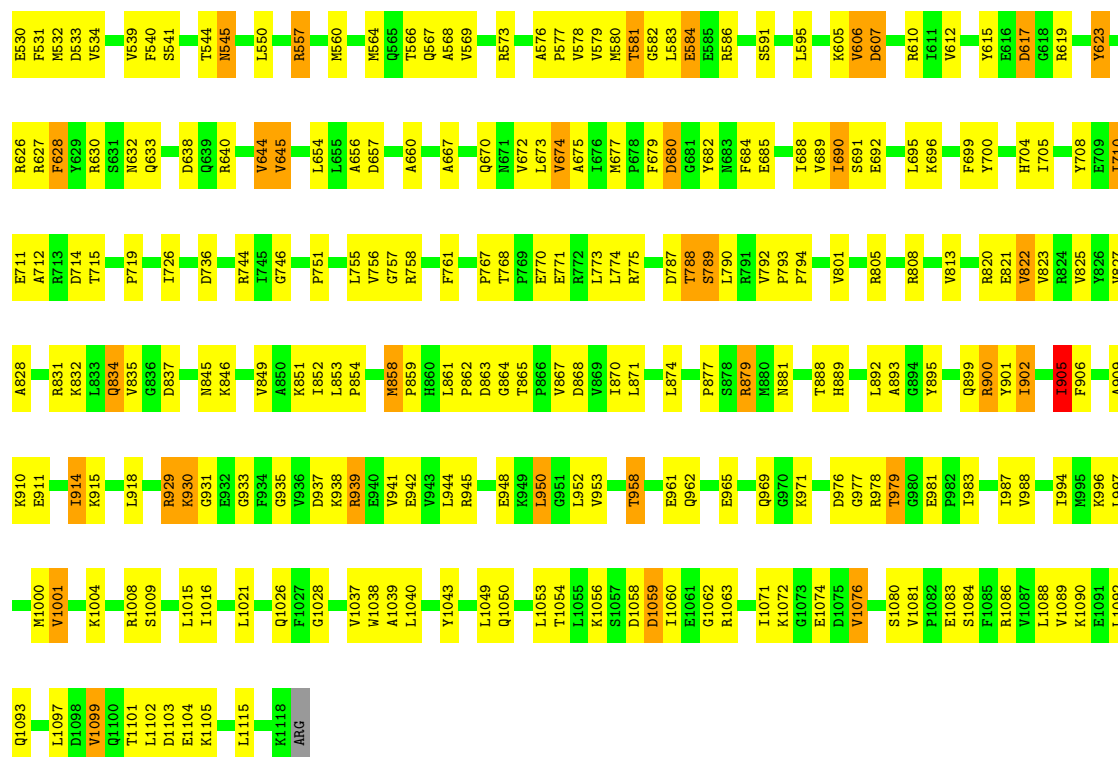


• Molecule 1: DNA-directed RNA polymerase subunit alpha



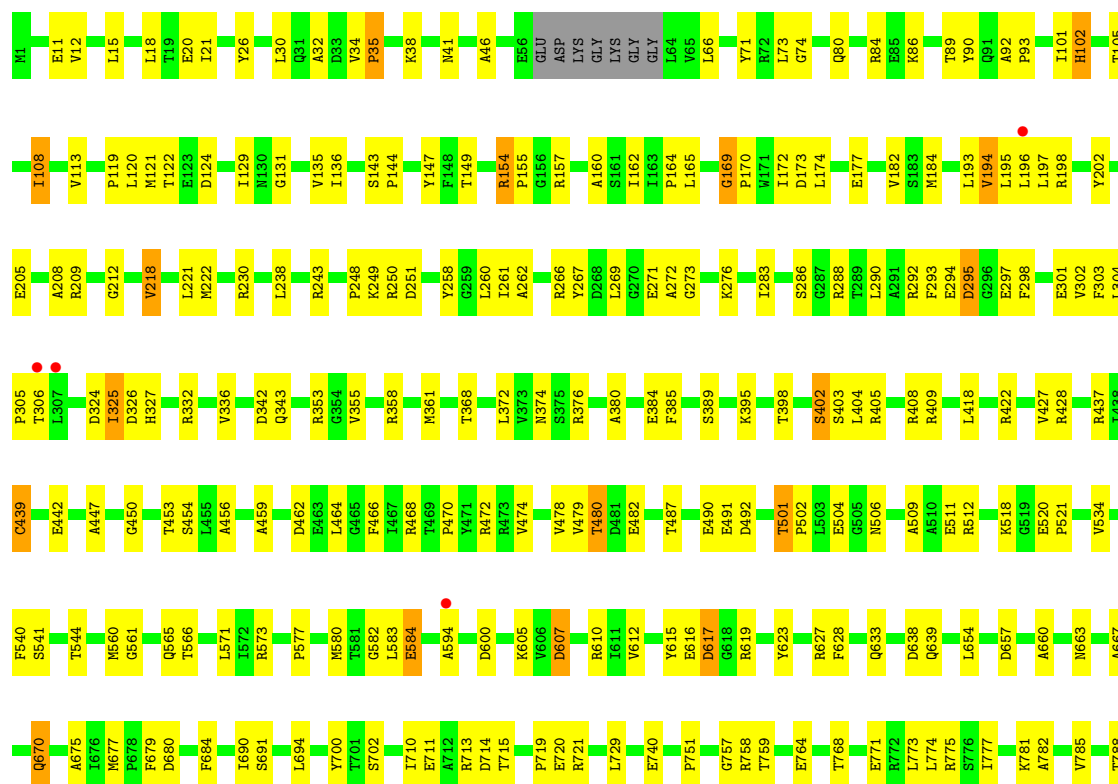
• Molecule 2: DNA-directed RNA polymerase subunit beta

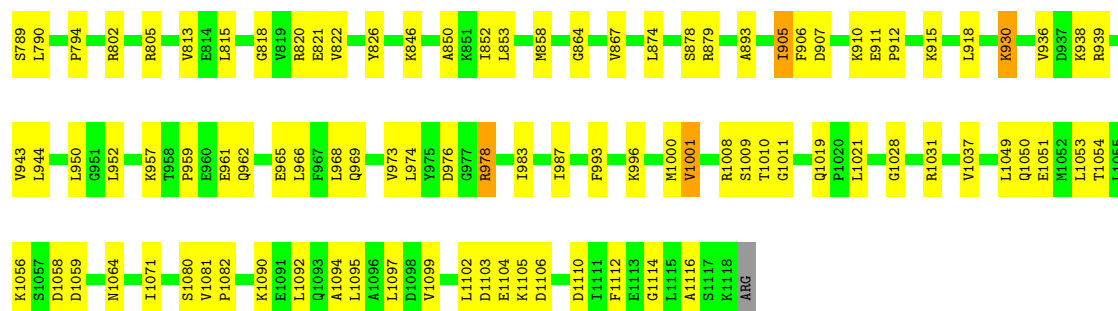




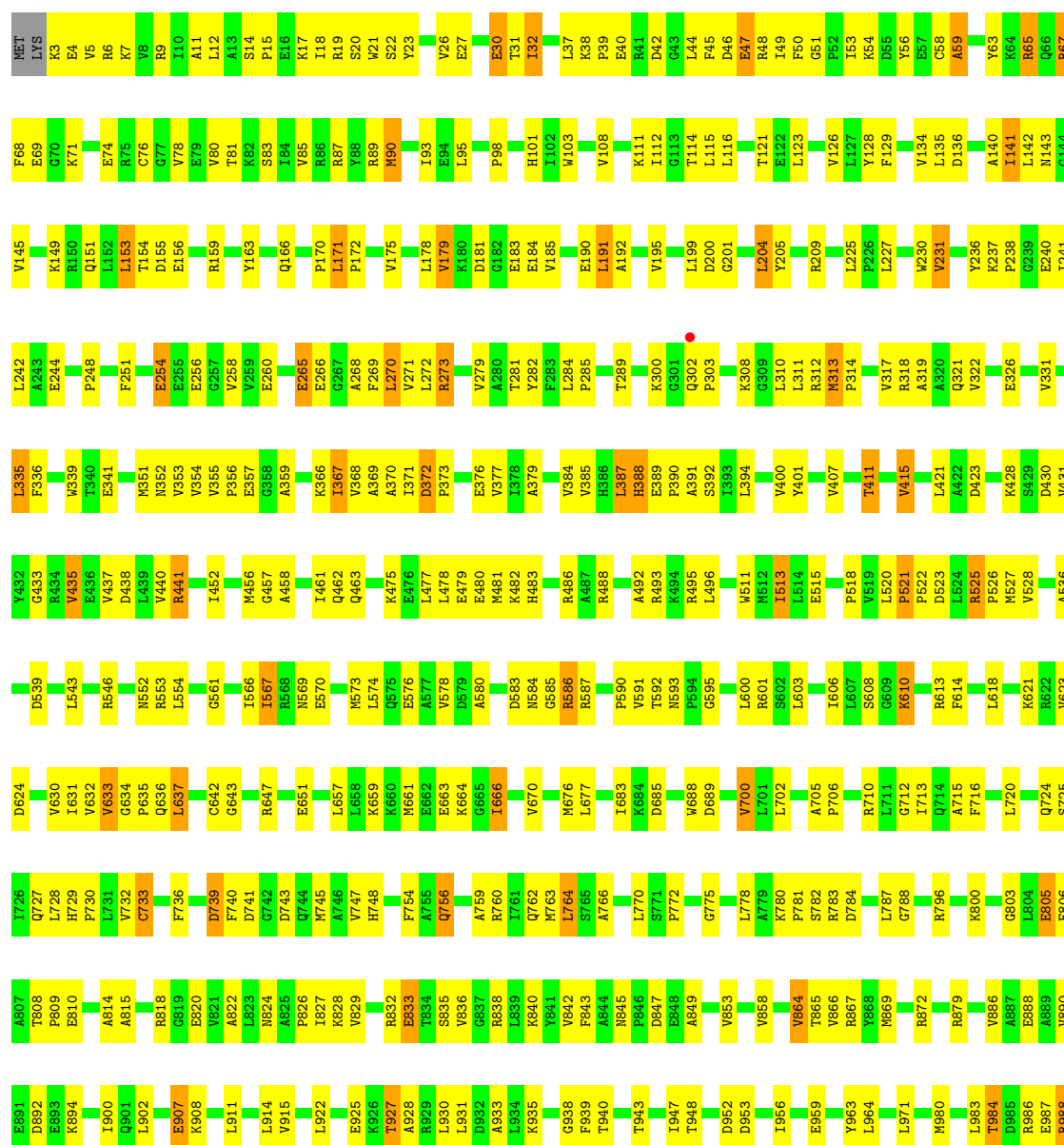
• Molecule 2: DNA-directed RNA polymerase subunit beta

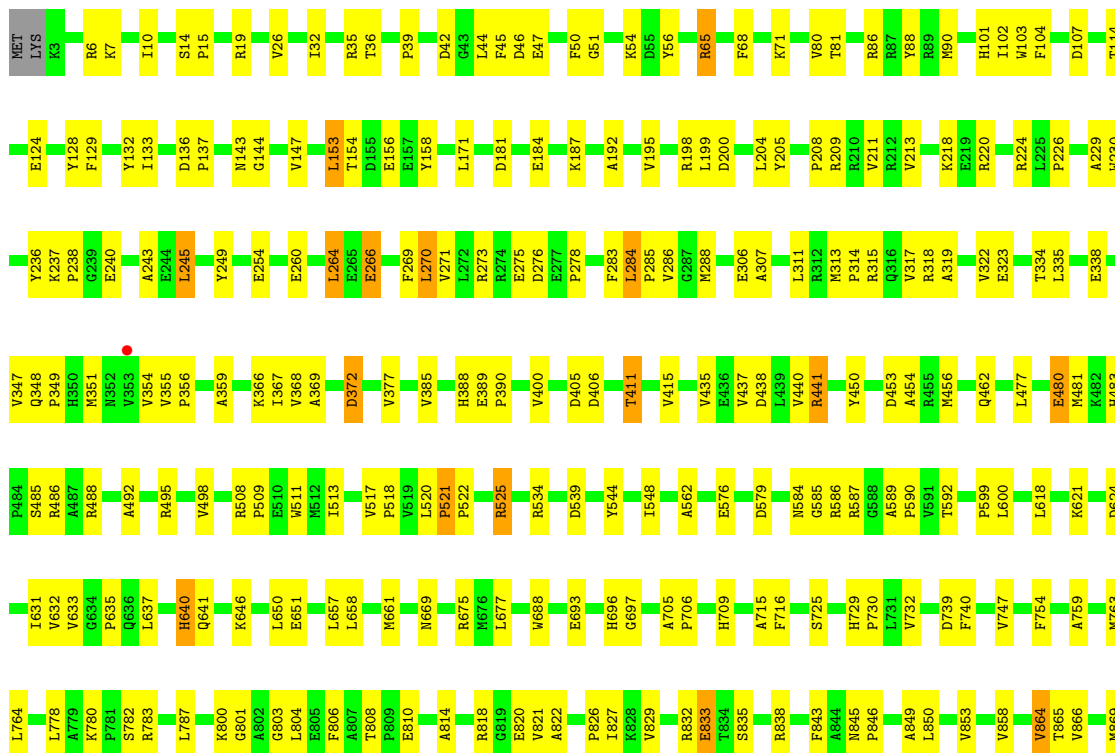
Chain M:  69%  28% ..

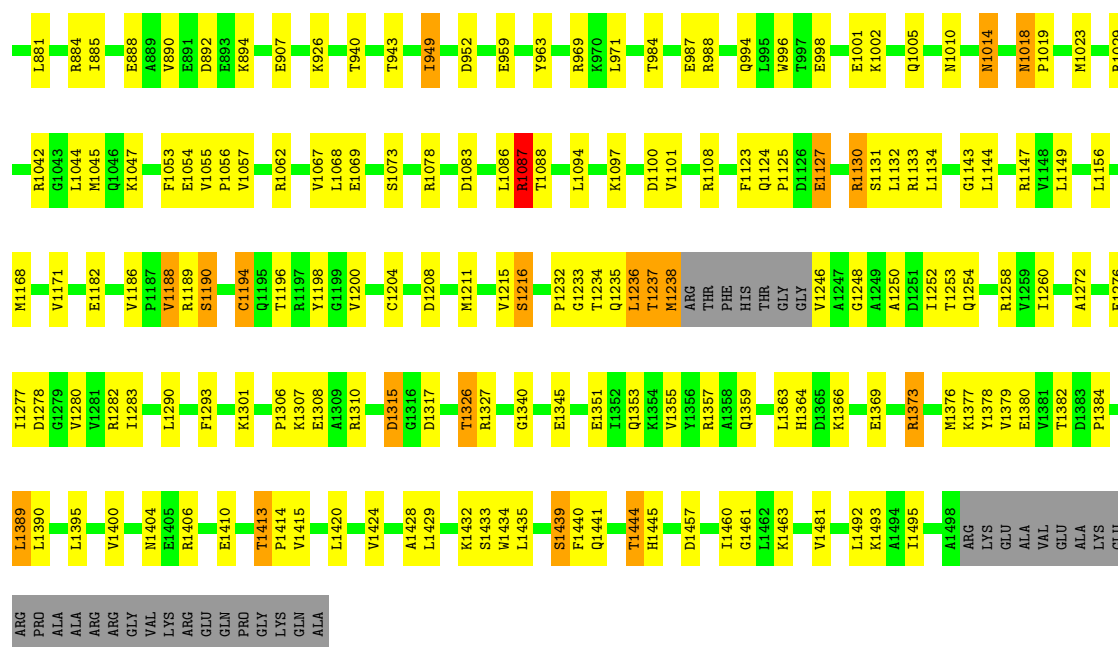




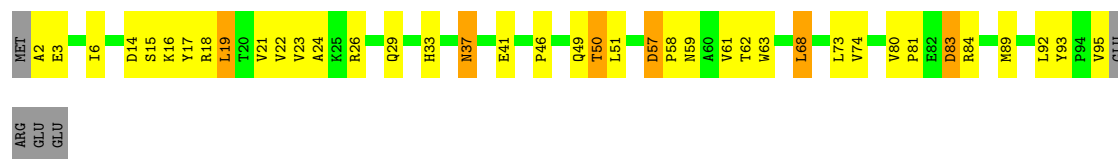
• Molecule 3: DNA-directed RNA polymerase subunit beta'







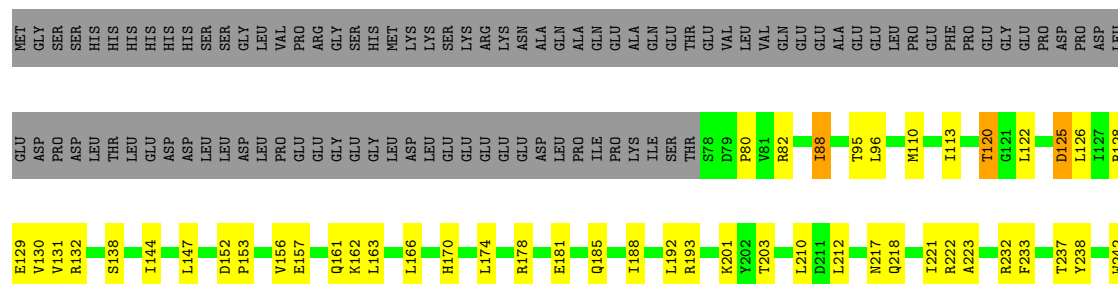
- Molecule 4: DNA-directed RNA polymerase subunit omega

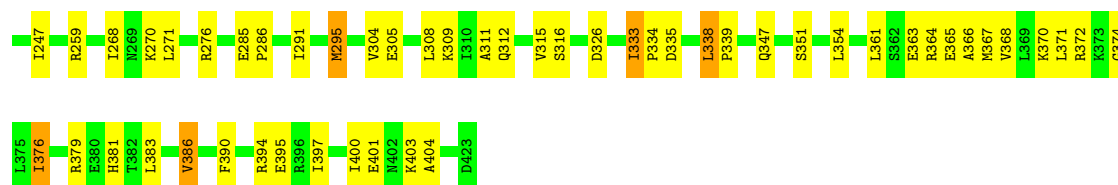


- Molecule 4: DNA-directed RNA polymerase subunit omega

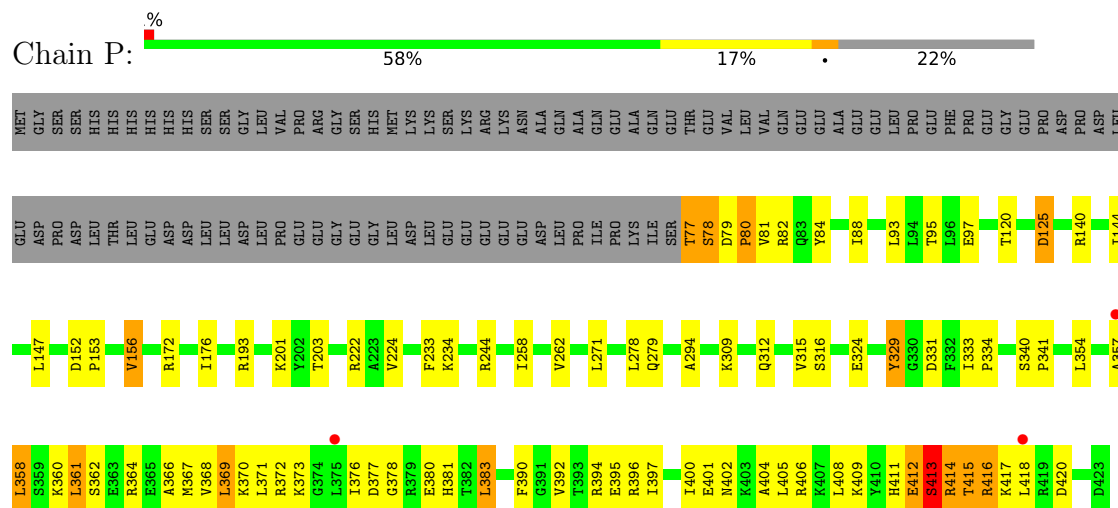


- Molecule 5: RNA polymerase sigma factor





- Molecule 5: RNA polymerase sigma factor



- Molecule 6: 5'-D(*TP*AP*TP*AP*AP*TP*GP*GP*GP*AP*GP*CP*TP*GP*TP*CP*AP*C
P*GP*GP*AP*TP*GP*CP*AP*GP*G)-3'



- Molecule 6: 5'-D(*TP*AP*TP*AP*AP*TP*GP*GP*GP*AP*GP*CP*TP*GP*TP*CP*AP*C
P*GP*GP*AP*TP*GP*CP*AP*GP*G)-3'



- Molecule 7: 5'-D(*CP*CP*TP*GP*CP*AP*TP*CP*CP*GP*TP*GP*AP*GP*(BRU)P*CP*
GP*AP*GP*GP*G)-3'



- Molecule 7: 5'-D(*CP*CP*TP*GP*CP*AP*TP*CP*CP*GP*TP*GP*AP*GP*(BRU)P*CP*
GP*AP*GP*GP*G)-3'



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	185.47Å 103.59Å 296.51Å 90.00° 98.53° 90.00°	Depositor
Resolution (Å)	49.85 – 3.81 49.85 – 3.81	Depositor EDS
% Data completeness (in resolution range)	51.6 (49.85-3.81) 81.7 (49.85-3.81)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	0.17	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.44 (at 3.77Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.176 , 0.232 0.193 , 0.251	Depositor DCC
R_{free} test set	1776 reflections (1.63%)	wwPDB-VP
Wilson B-factor (Å ²)	120.0	Xtriage
Anisotropy	0.137	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 107.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	56872	wwPDB-VP
Average B, all atoms (Å ²)	151.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 40.98 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.5249e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical 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

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

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	0.61	0/1814	1.10	14/2466 (0.6%)
1	B	0.60	0/1782	1.11	11/2424 (0.5%)
1	K	0.34	0/1814	0.84	4/2466 (0.2%)
1	L	0.34	0/1805	0.82	5/2454 (0.2%)
2	C	0.62	0/8937	1.08	40/12087 (0.3%)
2	M	0.35	0/8937	0.85	18/12087 (0.1%)
3	D	0.63	0/11910	1.08	59/16105 (0.4%)
3	N	0.34	0/11952	0.83	19/16162 (0.1%)
4	E	0.57	0/775	1.03	5/1045 (0.5%)
4	O	0.31	0/775	0.78	0/1045
5	F	0.35	0/2852	0.80	4/3837 (0.1%)
5	P	0.36	0/2859	0.79	2/3847 (0.1%)
6	H	0.37	0/556	1.06	0/858
6	R	0.41	0/556	1.04	1/858 (0.1%)
7	G	0.36	0/345	0.81	0/529
7	Q	0.34	0/345	0.75	0/529
All	All	0.49	0/58014	0.95	182/78799 (0.2%)

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
2	M	0	1

There are no bond length outliers.

All (182) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	8	ALA	CA-C-N	10.36	130.46	120.31
1	A	8	ALA	C-N-CA	10.36	130.46	120.31
2	C	398	THR	N-CA-C	-9.73	99.97	112.23
1	B	48	ILE	CA-C-N	8.93	128.87	119.85
1	B	48	ILE	C-N-CA	8.93	128.87	119.85
2	C	439	CYS	CA-C-N	8.63	130.63	119.84
2	C	439	CYS	C-N-CA	8.63	130.63	119.84
1	A	172	SER	CA-C-N	8.51	128.72	119.87
1	A	172	SER	C-N-CA	8.51	128.72	119.87
3	D	1018	ASN	CA-C-N	8.50	129.00	119.32
3	D	1018	ASN	C-N-CA	8.50	129.00	119.32
1	B	172	SER	CA-C-N	8.05	128.24	119.87
1	B	172	SER	C-N-CA	8.05	128.24	119.87
3	D	1120	VAL	N-CA-C	7.73	114.59	107.56
3	N	1340	GLY	CA-C-N	7.71	126.99	118.97
3	N	1340	GLY	C-N-CA	7.71	126.99	118.97
3	D	521	PRO	CA-C-N	7.68	127.39	119.56
3	D	521	PRO	C-N-CA	7.68	127.39	119.56
2	C	623	TYR	CA-C-N	-7.61	112.85	120.31
2	C	623	TYR	C-N-CA	-7.61	112.85	120.31
2	C	389	SER	N-CA-C	7.44	120.59	110.55
2	C	363	SER	N-CA-C	-7.39	98.95	109.96
2	C	169	GLY	CA-C-N	7.35	127.51	120.31
2	C	169	GLY	C-N-CA	7.35	127.51	120.31
1	B	8	ALA	CA-C-N	7.32	127.24	119.85
1	B	8	ALA	C-N-CA	7.32	127.24	119.85
1	A	95	GLN	N-CA-C	7.31	123.09	113.30
2	C	229	MET	N-CA-C	7.24	120.23	111.40
3	D	1144	LEU	N-CA-C	7.21	122.47	112.45
3	D	65	ARG	CB-CA-C	-7.17	107.25	115.79
1	K	8	ALA	CA-C-N	7.10	127.27	120.31
1	K	8	ALA	C-N-CA	7.10	127.27	120.31
3	D	1055	VAL	CA-C-N	6.97	127.53	120.14
3	D	1055	VAL	C-N-CA	6.97	127.53	120.14
3	D	1497	GLU	N-CA-C	6.93	118.73	111.03
3	D	1340	GLY	CA-C-N	6.89	127.17	119.32
3	D	1340	GLY	C-N-CA	6.89	127.17	119.32
1	K	172	SER	CA-C-N	6.83	126.98	119.87
1	K	172	SER	C-N-CA	6.83	126.98	119.87
2	C	690	ILE	N-CA-C	6.82	117.94	108.12
3	D	225	LEU	CA-C-N	6.79	126.83	119.90
3	D	225	LEU	C-N-CA	6.79	126.83	119.90
3	D	1472	ILE	CA-C-N	6.57	126.26	119.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1472	ILE	C-N-CA	6.57	126.26	119.82
2	C	858	MET	CA-C-N	6.53	126.92	119.93
2	C	858	MET	C-N-CA	6.53	126.92	119.93
1	B	140	MET	N-CA-C	6.45	118.66	108.79
4	E	41	GLU	CA-C-N	6.45	126.95	119.47
4	E	41	GLU	C-N-CA	6.45	126.95	119.47
2	C	410	ILE	CB-CA-C	-6.43	101.74	110.42
3	N	521	PRO	CA-C-N	6.37	126.28	119.28
3	N	521	PRO	C-N-CA	6.37	126.28	119.28
3	N	1186	VAL	N-CA-C	6.35	114.97	107.73
3	D	724	GLN	N-CA-C	6.34	120.71	112.92
3	D	1112	CYS	N-CA-C	-6.19	105.49	113.16
3	D	1413	THR	CA-C-N	6.16	126.35	120.31
3	D	1413	THR	C-N-CA	6.16	126.35	120.31
3	D	289	THR	CB-CA-C	-6.16	104.90	110.44
2	C	118	ILE	CA-C-N	6.14	126.16	119.90
2	C	118	ILE	C-N-CA	6.14	126.16	119.90
3	D	1256	LEU	CA-C-N	-6.13	112.70	119.19
3	D	1256	LEU	C-N-CA	-6.13	112.70	119.19
5	P	203	THR	N-CA-C	6.12	118.49	111.02
1	A	122	ILE	CB-CA-C	-6.09	103.52	111.25
1	L	172	SER	CA-C-N	6.07	125.75	119.56
1	L	172	SER	C-N-CA	6.07	125.75	119.56
2	M	439	CYS	CA-C-N	6.07	125.46	118.85
2	M	439	CYS	C-N-CA	6.07	125.46	118.85
2	C	118	ILE	N-CA-C	5.99	117.17	107.71
3	D	1328	GLY	N-CA-C	5.97	118.14	112.04
2	C	640	ARG	N-CA-C	-5.95	101.34	110.32
3	N	1190	SER	CA-C-N	5.94	126.36	119.47
3	N	1190	SER	C-N-CA	5.94	126.36	119.47
2	M	169	GLY	CA-C-N	5.93	126.12	120.31
2	M	169	GLY	C-N-CA	5.93	126.12	120.31
1	A	115	LEU	CA-C-N	5.91	126.22	119.83
1	A	115	LEU	C-N-CA	5.91	126.22	119.83
2	C	271	GLU	N-CA-C	-5.91	104.97	111.82
3	D	388	HIS	N-CA-C	5.83	120.03	111.34
2	M	501	THR	CA-C-N	5.81	125.74	119.76
2	M	501	THR	C-N-CA	5.81	125.74	119.76
3	D	1186	VAL	N-CA-C	5.80	116.87	107.71
3	D	136	ASP	CA-C-N	-5.79	113.05	119.19
3	D	136	ASP	C-N-CA	-5.79	113.05	119.19
2	M	154	ARG	CA-C-N	5.73	124.93	118.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	154	ARG	C-N-CA	5.73	124.93	118.97
3	D	614	PHE	N-CA-C	5.70	118.36	111.40
2	C	165	LEU	CA-C-N	5.68	125.79	119.32
2	C	165	LEU	C-N-CA	5.68	125.79	119.32
2	M	1081	VAL	N-CA-C	5.67	113.50	108.63
1	B	61	VAL	N-CA-C	5.66	116.01	107.80
5	P	78	SER	CB-CA-C	-5.65	110.08	116.63
3	N	313	MET	CA-C-N	-5.64	114.76	120.85
3	N	313	MET	C-N-CA	-5.64	114.76	120.85
3	D	833	GLU	N-CA-C	5.63	119.41	111.52
3	N	1018	ASN	CA-C-N	5.63	125.74	119.32
3	N	1018	ASN	C-N-CA	5.63	125.74	119.32
3	D	1313	VAL	N-CA-C	5.62	115.96	107.75
1	A	174	VAL	CB-CA-C	-5.61	105.17	111.23
2	M	1011	GLY	CA-C-N	5.61	125.53	119.76
2	M	1011	GLY	C-N-CA	5.61	125.53	119.76
3	N	65	ARG	CB-CA-C	-5.60	109.12	115.79
4	E	68	LEU	N-CA-C	5.60	117.38	111.28
3	N	229	ALA	N-CA-C	5.59	117.24	111.03
1	A	140	MET	N-CA-C	5.58	116.75	108.60
3	D	610	LYS	N-CA-C	-5.56	105.30	111.36
3	D	618	LEU	N-CA-C	5.54	119.22	112.23
3	D	5	VAL	CB-CA-C	-5.54	104.22	111.81
3	D	38	LYS	CA-C-N	5.52	125.83	119.93
3	D	38	LYS	C-N-CA	5.52	125.83	119.93
6	R	24	DC	O5'-C5'-C4'	5.51	119.07	110.80
1	L	48	ILE	CA-C-N	5.50	125.42	119.76
1	L	48	ILE	C-N-CA	5.50	125.42	119.76
3	D	59	ALA	N-CA-C	5.49	117.97	111.33
2	M	398	THR	N-CA-C	-5.47	104.17	112.04
2	C	3	ILE	CB-CA-C	-5.47	103.59	111.19
2	C	1076	VAL	N-CA-C	5.44	114.08	109.02
3	N	739	ASP	N-CA-C	-5.43	101.46	109.18
3	D	367	ILE	N-CA-C	5.42	116.91	111.00
5	F	203	THR	N-CA-C	5.41	117.62	111.02
3	N	833	GLU	N-CA-C	5.41	118.58	111.28
1	L	118	ALA	CB-CA-C	-5.40	110.33	116.54
2	M	271	GLU	N-CA-C	-5.40	105.56	111.82
4	E	57	ASP	CA-C-N	5.39	125.01	119.56
4	E	57	ASP	C-N-CA	5.39	125.01	119.56
3	D	1352	ILE	CB-CA-C	-5.39	104.92	111.87
2	C	410	ILE	N-CA-C	5.38	115.74	107.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1026	GLN	N-CA-C	-5.38	106.49	113.16
2	C	6	PHE	N-CA-C	5.35	117.78	110.55
1	A	142	VAL	N-CA-C	5.34	115.54	107.80
3	D	1458	GLU	CA-C-N	-5.32	115.46	122.85
3	D	1458	GLU	C-N-CA	-5.32	115.46	122.85
1	B	10	VAL	N-CA-C	5.32	115.23	107.37
2	C	1004	LYS	N-CA-C	5.32	118.93	112.23
2	C	988	VAL	CB-CA-C	-5.31	104.22	111.33
3	D	163	TYR	N-CA-C	5.30	119.85	113.17
3	D	313	MET	CA-C-N	5.30	125.77	120.52
3	D	313	MET	C-N-CA	5.30	125.77	120.52
2	C	163	ILE	N-CA-C	5.30	113.77	107.73
3	N	441	ARG	N-CA-C	-5.30	101.83	110.20
3	D	592	THR	N-CA-C	-5.29	105.59	111.36
1	B	165	ILE	CA-C-N	5.27	125.03	119.76
1	B	165	ILE	C-N-CA	5.27	125.03	119.76
2	C	373	VAL	N-CA-C	5.27	115.71	108.12
3	D	1101	VAL	CB-CA-C	-5.27	105.12	112.02
2	C	576	ALA	CA-C-N	5.26	125.27	119.90
2	C	576	ALA	C-N-CA	5.26	125.27	119.90
3	D	1474	ALA	N-CA-C	5.25	117.86	110.14
3	D	204	LEU	N-CA-C	5.25	117.36	109.23
3	D	634	GLY	N-CA-C	5.25	123.05	112.34
5	F	333	ILE	CA-C-N	5.24	125.22	120.03
5	F	333	ILE	C-N-CA	5.24	125.22	120.03
3	D	483	HIS	CA-C-N	5.23	124.41	118.97
3	D	483	HIS	C-N-CA	5.23	124.41	118.97
3	N	1014	ASN	N-CA-C	5.23	118.12	111.69
2	C	941	VAL	CB-CA-C	-5.22	105.18	112.02
2	C	914	ILE	CB-CA-C	-5.22	105.18	112.02
3	D	664	LYS	N-CA-C	-5.21	103.66	110.53
3	D	1410	GLU	N-CA-C	-5.20	106.62	113.17
2	M	243	ARG	CA-C-N	5.19	125.39	120.31
2	M	243	ARG	C-N-CA	5.19	125.39	120.31
2	M	303	PHE	N-CA-C	5.17	116.92	111.28
3	D	836	VAL	CB-CA-C	-5.17	105.27	112.04
3	D	515	GLU	N-CA-C	-5.17	105.05	112.13
2	C	303	PHE	N-CA-C	5.17	116.99	111.36
1	A	48	ILE	CA-C-N	5.16	125.60	120.14
1	A	48	ILE	C-N-CA	5.16	125.60	120.14
5	F	326	ASP	N-CA-C	5.15	117.79	111.82
2	C	905	ILE	CB-CA-C	-5.14	103.20	111.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	N	284	LEU	CA-C-N	5.14	125.35	120.31
3	N	284	LEU	C-N-CA	5.14	125.35	120.31
2	M	35	PRO	CA-C-N	5.14	125.44	119.47
2	M	35	PRO	C-N-CA	5.14	125.44	119.47
2	C	35	PRO	CA-C-N	5.13	125.42	119.47
2	C	35	PRO	C-N-CA	5.13	125.42	119.47
2	C	688	ILE	N-CA-C	5.13	116.04	108.45
1	A	26	GLU	N-CA-C	5.09	116.47	108.23
3	D	739	ASP	CA-C-N	-5.06	115.28	123.23
3	D	739	ASP	C-N-CA	-5.06	115.28	123.23
3	D	595	GLY	N-CA-C	5.06	118.76	112.64
2	C	1059	ASP	N-CA-C	-5.03	100.87	108.67
3	D	384	VAL	N-CA-C	5.00	115.32	108.12

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	M	294	GLU	Peptide

5.2 Too-close contacts

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	1782	0	1834	71	0
1	B	1750	0	1797	67	0
1	K	1782	0	1834	32	0
1	L	1773	0	1826	37	0
2	C	8770	0	8874	320	0
2	M	8770	0	8874	217	0
3	D	11704	0	11934	408	0
3	N	11746	0	11974	284	0
4	E	761	0	778	32	0
4	O	761	0	778	20	0
5	F	2807	0	2882	74	0
5	P	2814	0	2889	123	0
6	H	495	0	272	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	R	495	0	272	16	0
7	G	328	0	178	7	0
7	Q	328	0	178	13	0
8	D	2	0	0	0	0
8	N	2	0	0	0	0
9	D	1	0	0	0	0
9	N	1	0	0	0	0
All	All	56872	0	57174	1572	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 14.

All (1572) 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)
5:P:408:LEU:O	5:P:412:GLU:CB	1.72	1.37
5:P:408:LEU:O	5:P:412:GLU:HB2	1.07	1.23
5:P:408:LEU:HD23	5:P:412:GLU:CG	1.69	1.21
7:Q:14:DG:H2''	7:Q:15:BRU:O5'	1.43	1.15
3:N:1238:MET:SD	3:N:1359:GLN:OE1	2.07	1.12
3:N:1238:MET:O	3:N:1246:VAL:HA	1.50	1.10
3:N:1238:MET:HE3	3:N:1238:MET:HA	1.10	1.09
3:N:1238:MET:HA	3:N:1238:MET:CE	1.84	1.07
3:D:1194:CYS:HB2	3:D:1204:CYS:SG	2.01	1.01
5:P:415:THR:HG22	5:P:416:ARG:HG2	1.40	1.00
5:P:77:THR:CG2	5:P:78:SER:N	2.30	0.95
3:N:1258:ARG:HH21	3:N:1351:GLU:HG2	1.33	0.91
5:P:408:LEU:HD23	5:P:412:GLU:HG3	1.50	0.90
5:P:408:LEU:HA	5:P:412:GLU:HG2	1.50	0.90
5:P:77:THR:CG2	5:P:78:SER:H	1.83	0.90
5:P:415:THR:CG2	5:P:416:ARG:HG2	2.03	0.88
5:P:416:ARG:O	5:P:417:LYS:HG2	1.72	0.88
2:C:757:GLY:HA2	2:C:789:SER:HB3	1.57	0.87
5:P:77:THR:HG22	5:P:78:SER:N	1.87	0.87
3:N:1238:MET:HE3	3:N:1238:MET:CA	2.01	0.87
5:P:412:GLU:HA	5:P:412:GLU:OE1	1.74	0.86
5:P:77:THR:HG23	5:P:78:SER:H	1.39	0.85
2:M:615:TYR:HH	2:M:623:TYR:HH	1.25	0.84
5:P:408:LEU:O	5:P:412:GLU:CG	2.25	0.84
1:L:90:LEU:HB2	1:L:119:ASP:HB3	1.59	0.84
5:P:408:LEU:HD23	5:P:412:GLU:CB	2.07	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:441:VAL:HG21	2:C:544:THR:HG21	1.58	0.83
2:M:764:GLU:HG2	3:N:54:LYS:HE2	1.60	0.83
3:N:592:THR:HB	3:N:600:LEU:HD21	1.59	0.83
3:N:800:LYS:HB3	3:N:822:ALA:HB2	1.60	0.83
5:P:408:LEU:HD23	5:P:412:GLU:HG2	1.60	0.83
3:D:988:ARG:NH2	3:D:1054:GLU:OE2	2.12	0.83
1:A:216:GLU:OE2	1:A:219:ARG:NH2	2.12	0.82
7:Q:14:DG:H2''	7:Q:15:BRU:C5'	2.08	0.82
3:D:260:GLU:OE1	3:D:273:ARG:NH1	2.12	0.82
5:P:408:LEU:C	5:P:412:GLU:HB2	2.04	0.82
5:P:411:HIS:O	5:P:415:THR:HG21	1.80	0.82
1:B:58:ILE:HB	1:B:61:VAL:HB	1.62	0.81
3:N:520:LEU:O	3:N:525:ARG:NH1	2.13	0.81
5:P:408:LEU:CA	5:P:412:GLU:HG2	2.10	0.80
2:M:628:PHE:H	2:M:638:ASP:HB3	1.47	0.80
3:D:739:ASP:OD1	3:D:741:ASP:CG	2.24	0.80
3:D:238:PRO:HD3	3:D:318:ARG:HG3	1.61	0.79
3:D:984:THR:HB	3:D:987:GLU:H	1.46	0.79
2:C:1050:GLN:O	2:C:1054:THR:OG1	1.99	0.79
5:P:411:HIS:O	5:P:415:THR:CB	2.30	0.79
2:M:266:ARG:NH1	6:R:11:DG:N7	2.31	0.79
1:B:206:THR:HG22	1:B:209:GLU:H	1.47	0.79
2:C:691:SER:HA	2:C:858:MET:HE3	1.64	0.79
3:D:1353:GLN:HE22	3:D:1363:LEU:HB3	1.48	0.78
3:D:520:LEU:O	3:D:525:ARG:NH1	2.17	0.77
2:M:324:ASP:HB3	2:M:327:HIS:HB2	1.65	0.77
3:N:1238:MET:O	3:N:1246:VAL:CA	2.30	0.77
2:C:395:LYS:HE2	2:C:403:SER:HB2	1.64	0.77
3:D:1341:PRO:HB3	3:D:1376:MET:HE1	1.66	0.77
2:M:212:GLY:HA2	2:M:218:VAL:HG21	1.67	0.77
2:M:617:ASP:HB2	2:M:619:ARG:HG2	1.66	0.76
2:C:573:ARG:O	2:C:670:GLN:NE2	2.17	0.76
3:D:657:LEU:HG	3:D:661:MET:HE2	1.67	0.76
3:D:576:GLU:OE2	3:D:587:ARG:NH1	2.17	0.76
5:P:412:GLU:OE1	5:P:412:GLU:CA	2.34	0.76
7:Q:15:BRU:N3	7:Q:16:DC:C5	2.54	0.76
2:C:877:PRO:HG3	3:D:1023:MET:HE1	1.68	0.75
1:B:57:TYR:HE1	1:B:163:ASN:HB2	1.52	0.75
2:C:1053:LEU:HA	3:D:621:LYS:HD2	1.68	0.75
3:N:39:PRO:HG2	3:N:47:GLU:HG3	1.68	0.75
3:D:26:VAL:HG11	3:D:44:LEU:HD23	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:206:THR:HG22	1:L:209:GLU:H	1.50	0.75
2:C:564:MET:HE1	2:C:846:LYS:HB3	1.68	0.74
3:D:1274:ILE:HD11	3:D:1334:GLN:HB3	1.69	0.74
5:F:386:VAL:HB	5:F:397:ILE:HG12	1.67	0.74
3:D:372:ASP:N	3:D:372:ASP:OD1	2.20	0.74
5:F:397:ILE:HD12	5:F:400:ILE:HD11	1.68	0.74
2:M:853:LEU:HB2	2:M:858:MET:HE1	1.68	0.74
3:N:1404:ASN:HD21	3:N:1415:VAL:H	1.33	0.74
2:M:950:LEU:HB3	2:M:952:LEU:HD13	1.70	0.74
2:C:394:PHE:HE2	2:C:632:ASN:HB3	1.53	0.73
2:C:353:ARG:HH22	6:H:9:DG:H3'	1.54	0.73
5:P:79:ASP:OD2	6:R:8:DG:N1	2.20	0.73
2:C:615:TYR:OH	2:C:623:TYR:OH	2.05	0.73
3:N:218:LYS:HG2	3:N:338:GLU:HG2	1.71	0.73
2:C:660:ALA:HB1	2:C:667:ALA:O	1.88	0.73
2:M:711:GLU:HG2	2:M:822:VAL:HG22	1.70	0.73
5:F:364:ARG:HH11	5:F:400:ILE:HD12	1.52	0.73
2:C:15:LEU:HD21	2:C:457:ALA:HB1	1.68	0.73
3:D:1435:LEU:O	3:D:1439:SER:OG	2.07	0.73
2:C:84:ARG:HA	2:C:131:GLY:HA2	1.71	0.73
6:H:21:DA:H61	7:G:7:DT:H3	1.37	0.73
2:C:86:LYS:HD3	2:C:813:VAL:HB	1.70	0.72
2:C:617:ASP:HB2	2:C:619:ARG:HG2	1.71	0.72
1:B:53:VAL:HG11	1:B:82:LEU:HD22	1.71	0.72
3:D:438:ASP:OD1	3:D:441:ARG:NH2	2.23	0.71
3:N:1404:ASN:ND2	3:N:1415:VAL:H	1.86	0.71
2:M:160:ALA:HB3	2:M:174:LEU:HB2	1.71	0.71
3:D:1315:ASP:OD1	3:D:1315:ASP:N	2.23	0.71
3:D:1406:ARG:O	3:D:1410:GLU:HB2	1.90	0.71
2:C:708:TYR:HE1	2:C:827:VAL:HB	1.55	0.71
3:D:14:SER:HB3	3:D:511:TRP:CE2	2.26	0.71
3:N:1395:LEU:HD11	3:N:1400:VAL:HB	1.71	0.71
2:C:1081:VAL:HB	2:C:1086:ARG:HH21	1.56	0.71
5:P:412:GLU:O	5:P:413:SER:C	2.33	0.71
3:D:1047:LYS:HB2	3:D:1051:GLU:O	1.90	0.71
3:N:411:THR:HB	3:N:437:VAL:H	1.54	0.71
3:N:1123:PHE:HB3	3:N:1132:LEU:HD21	1.73	0.71
2:C:1102:LEU:HB2	3:D:7:LYS:HB2	1.73	0.71
5:P:392:VAL:HG21	5:P:397:ILE:HD13	1.73	0.71
1:A:42:ARG:NH2	1:B:31:GLY:O	2.23	0.70
2:C:134:ARG:NH1	2:C:392:SER:O	2.23	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1152:GLU:HG2	3:D:1161:GLU:HA	1.72	0.70
3:N:1435:LEU:O	3:N:1439:SER:OG	2.09	0.70
3:D:411:THR:HB	3:D:437:VAL:H	1.56	0.70
2:M:1110:ASP:OD2	2:M:1114:GLY:N	2.25	0.70
3:N:669:ASN:HD22	5:P:417:LYS:HD2	1.55	0.70
1:K:30:ARG:HD3	1:K:191:ASP:HB2	1.72	0.70
2:C:470:PRO:HB2	2:C:534:VAL:HG21	1.74	0.70
5:F:400:ILE:HA	5:F:403:LYS:HG2	1.71	0.70
5:P:411:HIS:O	5:P:415:THR:CG2	2.39	0.70
3:N:1232:PRO:O	3:N:1235:GLN:HB2	1.91	0.69
5:P:408:LEU:CD2	5:P:412:GLU:CG	2.62	0.69
7:Q:14:DG:C2'	7:Q:15:BRU:O5'	2.30	0.69
3:D:1480:PHE:O	4:E:18:ARG:NH2	2.25	0.69
1:B:80:LEU:HD23	3:D:867:ARG:HD3	1.75	0.69
6:R:21:DA:H61	7:Q:7:DT:H3	1.38	0.69
1:K:39:PRO:HG3	1:L:39:PRO:HG3	1.75	0.69
2:M:773:LEU:HD23	5:P:354:LEU:HD13	1.74	0.69
5:P:408:LEU:O	5:P:412:GLU:CA	2.40	0.68
2:M:714:ASP:OD1	2:M:820:ARG:NH2	2.22	0.68
3:N:372:ASP:OD1	3:N:372:ASP:N	2.25	0.68
2:M:102:HIS:HB3	2:M:105:THR:HB	1.74	0.68
2:C:684:PHE:HB3	3:D:633:VAL:HG21	1.75	0.68
3:D:864:VAL:HG12	3:D:865:THR:H	1.58	0.68
3:N:1237:THR:O	3:N:1238:MET:HB2	1.94	0.68
3:D:68:PHE:HB3	3:D:71:LYS:HB3	1.75	0.68
3:D:843:PHE:HB2	3:D:866:VAL:HG22	1.75	0.68
2:M:66:LEU:HD22	2:M:372:LEU:HD23	1.75	0.68
2:M:1092:LEU:HD13	2:M:1099:VAL:HG21	1.76	0.68
3:N:323:GLU:HB2	3:N:334:THR:HB	1.75	0.68
3:N:988:ARG:NH2	3:N:1054:GLU:OE2	2.27	0.68
3:N:1495:ILE:HG12	4:O:88:GLU:HG3	1.74	0.68
5:P:144:ILE:HB	5:P:147:LEU:HB2	1.75	0.67
2:C:1037:VAL:HG13	2:C:1049:LEU:HD11	1.74	0.67
2:C:950:LEU:HB3	2:C:952:LEU:HD13	1.74	0.67
3:N:124:GLU:OE2	3:N:587:ARG:NH2	2.27	0.67
2:C:30:LEU:O	2:C:71:TYR:OH	2.12	0.67
2:M:893:ALA:HB2	2:M:918:LEU:HD23	1.76	0.67
2:C:15:LEU:O	2:C:586:ARG:NH2	2.22	0.67
2:M:521:PRO:HB3	3:N:1068:LEU:HD21	1.76	0.67
1:A:30:ARG:HD3	1:A:191:ASP:HB2	1.74	0.67
1:B:77:GLU:O	1:B:81:ASN:ND2	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:994:GLN:NE2	3:D:998:GLU:OE2	2.26	0.67
3:N:1238:MET:HG3	3:N:1253:THR:HB	1.77	0.67
3:D:1128:VAL:HG23	3:D:1133:ARG:HD3	1.76	0.66
3:N:1083:ASP:O	3:N:1087:ARG:CG	2.43	0.66
3:D:1147:ARG:HD3	3:D:1188:VAL:HG11	1.77	0.66
3:D:496:LEU:HD23	3:D:1390:LEU:HD13	1.77	0.66
2:M:395:LYS:HE2	2:M:403:SER:HB2	1.78	0.66
3:N:657:LEU:HG	3:N:661:MET:HE2	1.76	0.66
2:C:266:ARG:NH2	6:H:11:DG:O6	2.28	0.66
2:C:617:ASP:OD1	2:C:617:ASP:N	2.28	0.66
5:P:79:ASP:O	5:P:81:VAL:N	2.29	0.66
2:M:577:PRO:HG2	2:M:580:MET:HG2	1.78	0.66
3:N:347:VAL:HG13	3:N:351:MET:HG3	1.77	0.66
3:D:1042:ARG:HB3	3:D:1057:VAL:HB	1.78	0.66
1:L:56:VAL:HG21	1:L:82:LEU:HD13	1.77	0.66
5:P:367:MET:HB3	5:P:390:PHE:HZ	1.60	0.66
1:A:43:ILE:HD11	1:A:218:LEU:HD13	1.78	0.65
2:C:1104:GLU:HB3	3:D:6:ARG:HG3	1.79	0.65
7:Q:14:DG:C2'	7:Q:15:BRU:H6	2.26	0.65
2:M:511:GLU:HG3	2:M:512:ARG:HG2	1.78	0.65
3:D:835:SER:HB3	3:D:838:ARG:HG3	1.77	0.65
2:M:573:ARG:O	2:M:670:GLN:NE2	2.30	0.65
3:D:155:ASP:OD2	3:D:159:ARG:NH1	2.29	0.65
3:D:553:ARG:HD2	3:D:570:GLU:OE2	1.97	0.65
2:M:802:ARG:HB2	2:M:826:TYR:HB2	1.79	0.65
1:B:185:ARG:HH11	1:B:190:THR:HG23	1.62	0.65
3:N:1233:GLY:O	3:N:1235:GLN:N	2.30	0.65
2:M:710:ILE:HD12	2:M:790:LEU:HB2	1.79	0.65
5:P:368:VAL:HG11	5:P:397:ILE:HD11	1.79	0.64
3:D:1465:ASN:OD1	3:D:1470:ARG:NH1	2.30	0.64
1:L:185:ARG:HH11	1:L:190:THR:HG23	1.61	0.64
3:D:285:PRO:HG2	3:D:311:LEU:HD12	1.78	0.64
3:D:326:GLU:HG2	3:D:331:VAL:HG22	1.79	0.64
3:D:1309:ALA:HB1	3:D:1326:THR:HG23	1.80	0.64
2:C:425:PHE:HD1	3:D:1079:LYS:HG3	1.62	0.64
5:P:408:LEU:CD2	5:P:412:GLU:HG3	2.24	0.64
3:D:1290:LEU:HD12	3:D:1307:LYS:HA	1.79	0.64
5:F:367:MET:HB3	5:F:390:PHE:HZ	1.62	0.64
5:F:163:LEU:HD13	5:F:174:LEU:HD13	1.79	0.63
1:L:44:LEU:HA	1:L:48:ILE:HD13	1.79	0.63
2:M:164:PRO:HA	2:M:269:LEU:HD12	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:492:ASP:HB3	2:M:518:LYS:HG2	1.79	0.63
2:C:770:GLU:OE2	5:F:351:SER:OG	2.16	0.63
2:C:567:GLN:HB2	2:C:997:LEU:HD22	1.79	0.63
2:C:1054:THR:O	2:C:1059:ASP:HB3	1.99	0.63
3:D:1254:GLN:HB3	3:D:1258:ARG:HB2	1.79	0.63
5:F:144:ILE:HB	5:F:147:LEU:HB2	1.81	0.63
3:N:1310:ARG:HD3	3:N:1327:ARG:HH11	1.64	0.63
2:M:1104:GLU:HB3	3:N:6:ARG:HG3	1.81	0.63
5:P:415:THR:HG22	5:P:416:ARG:N	2.13	0.63
2:M:12:VAL:HG11	2:M:472:ARG:HD3	1.81	0.63
3:N:1208:ASP:HB2	3:N:1215:VAL:HA	1.81	0.63
1:B:201:THR:HG21	1:B:205:VAL:O	1.99	0.62
3:D:959:GLU:HB3	3:D:963:TYR:CE1	2.33	0.62
2:M:1008:ARG:HH11	2:M:1028:GLY:HA2	1.63	0.62
2:C:937:ASP:OD2	2:C:939:ARG:NH1	2.32	0.62
4:E:59:ASN:HB3	4:E:62:THR:OG1	1.99	0.62
5:P:408:LEU:O	5:P:412:GLU:N	2.31	0.62
6:R:2:DA:C8	6:R:2:DA:H5'	2.34	0.62
2:C:283:ILE:HD13	2:C:305:PRO:HG2	1.81	0.62
2:C:1103:ASP:HB3	2:C:1105:LYS:H	1.63	0.62
3:D:321:GLN:HB2	3:D:336:PHE:HD2	1.64	0.62
3:D:584:ASN:ND2	3:D:590:PRO:HD2	2.15	0.62
3:N:835:SER:HB3	3:N:838:ARG:HG3	1.82	0.62
5:P:79:ASP:OD2	5:P:82:ARG:HB2	1.98	0.62
1:L:58:ILE:HB	1:L:61:VAL:HB	1.82	0.62
3:N:266:GLU:OE2	3:N:315:ARG:NH2	2.33	0.62
2:C:168:ARG:NH2	2:C:265:ARG:O	2.29	0.62
3:D:154:THR:HG22	3:D:156:GLU:H	1.64	0.62
3:N:260:GLU:OE1	3:N:273:ARG:NH1	2.33	0.62
3:N:1100:ASP:OD1	3:N:1463:LYS:NZ	2.28	0.62
1:A:39:PRO:HG3	1:B:39:PRO:HG3	1.82	0.62
1:B:212:ASN:HA	1:B:215:VAL:HG22	1.82	0.62
3:D:9:ARG:HG3	3:D:1456:LYS:HG3	1.81	0.62
6:H:15:DT:H2''	6:H:16:DC:H5'	1.81	0.62
3:N:438:ASP:OD1	3:N:441:ARG:NH2	2.28	0.62
3:N:1127:GLU:HG3	3:N:1133:ARG:HB3	1.81	0.62
5:P:78:SER:O	5:P:79:ASP:C	2.43	0.62
3:D:539:ASP:OD1	5:F:316:SER:OG	2.18	0.62
3:D:590:PRO:HB2	3:D:600:LEU:HD12	1.82	0.61
1:A:58:ILE:HB	1:A:61:VAL:HB	1.82	0.61
2:C:607:ASP:HB3	2:C:610:ARG:H	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:39:PRO:HB3	3:D:45:PHE:O	2.00	0.61
3:D:661:MET:HE1	3:D:677:LEU:HD11	1.81	0.61
2:C:404:LEU:HD13	2:C:591:SER:HB2	1.80	0.61
3:D:890:VAL:HG23	3:D:892:ASP:H	1.65	0.61
2:M:258:TYR:HB2	2:M:298:PHE:HZ	1.65	0.61
7:Q:14:DG:C4	7:Q:15:BRU:BR	3.08	0.61
3:N:1233:GLY:C	3:N:1235:GLN:H	2.08	0.61
3:N:224:ARG:NE	3:N:254:GLU:OE2	2.25	0.61
1:A:135:GLY:O	1:A:137:ARG:HG3	2.01	0.61
3:D:15:PRO:HA	3:D:18:ILE:HD12	1.83	0.61
1:B:59:GLU:OE1	1:B:139:ASN:ND2	2.26	0.61
2:C:32:ALA:HB2	2:C:73:LEU:HD12	1.81	0.61
3:D:355:VAL:HG11	3:D:385:VAL:HG21	1.81	0.61
2:M:691:SER:HA	2:M:858:MET:HE3	1.83	0.61
2:C:893:ALA:HB2	2:C:918:LEU:HD23	1.82	0.61
3:D:1353:GLN:NE2	3:D:1363:LEU:HB3	2.15	0.61
3:D:1405:GLU:HA	3:D:1408:ILE:HG22	1.82	0.61
1:B:44:LEU:HA	1:B:48:ILE:HD13	1.82	0.60
1:B:138:LEU:HD11	1:B:140:MET:HE3	1.81	0.60
2:C:394:PHE:CE2	2:C:632:ASN:HB3	2.36	0.60
3:D:775:GLY:HA2	3:D:1209:LEU:HB3	1.83	0.60
3:D:1127:GLU:HB3	3:D:1133:ARG:HE	1.65	0.60
1:A:133:GLU:OE2	2:C:605:LYS:HA	2.01	0.60
5:F:238:TYR:HH	6:H:1:DT:H6	1.50	0.60
1:B:77:GLU:HB2	3:D:872:ARG:NH1	2.16	0.60
3:N:832:ARG:HG3	3:N:833:GLU:HG2	1.83	0.60
5:P:364:ARG:O	5:P:368:VAL:HG13	2.01	0.60
3:D:1285:GLU:HA	3:D:1290:LEU:HD23	1.83	0.60
3:N:1083:ASP:OD1	3:N:1087:ARG:NH1	2.35	0.60
3:D:716:PHE:HZ	3:D:732:VAL:HG21	1.67	0.60
3:D:988:ARG:HH11	3:D:988:ARG:HB3	1.65	0.60
4:E:26:ARG:NH1	4:E:29:GLN:OE1	2.33	0.60
3:N:808:THR:HG22	3:N:810:GLU:H	1.66	0.60
5:P:415:THR:CG2	5:P:416:ARG:N	2.64	0.60
5:P:409:LYS:HG2	5:P:413:SER:HB2	1.84	0.60
3:D:112:ILE:HB	3:D:123:LEU:HD21	1.84	0.60
2:C:12:VAL:HG11	2:C:472:ARG:HD3	1.83	0.60
3:N:1130:ARG:HD3	3:N:1131:SER:H	1.67	0.60
5:P:408:LEU:O	5:P:412:GLU:HG2	2.01	0.60
1:K:179:PHE:HB3	1:K:197:LEU:HD23	1.83	0.60
3:N:366:LYS:HD3	3:N:369:ALA:HB2	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:THR:HB	1:A:209:GLU:HG3	1.84	0.60
2:C:690:ILE:HB	2:C:852:ILE:HD13	1.84	0.60
3:N:270:LEU:HD23	3:N:284:LEU:HD11	1.83	0.60
3:N:1429:LEU:HG	3:N:1440:PHE:HD1	1.66	0.60
2:C:540:PHE:HE1	2:C:906:PHE:HE2	1.50	0.59
2:M:198:ARG:HH11	2:M:230:ARG:HA	1.67	0.59
2:M:617:ASP:OD1	2:M:617:ASP:N	2.35	0.59
2:C:704:HIS:HD2	2:C:831:ARG:HG3	1.67	0.59
3:D:580:ALA:O	3:D:584:ASN:HB2	2.02	0.59
3:D:268:ALA:HB3	3:D:284:LEU:HB2	1.82	0.59
1:L:71:VAL:HG22	1:L:132:LEU:HG	1.84	0.59
2:M:402:SER:HA	2:M:566:THR:HG23	1.83	0.59
3:D:1216:SER:HB3	4:E:16:LYS:H	1.66	0.59
2:M:86:LYS:HD2	2:M:813:VAL:HB	1.84	0.59
2:M:1001:VAL:HG11	3:N:725:SER:HB3	1.83	0.59
1:A:83:LYS:HE2	1:A:168:ASP:HB2	1.84	0.59
2:C:324:ASP:HB3	2:C:327:HIS:HB2	1.82	0.59
2:M:983:ILE:HG21	2:M:987:ILE:HD11	1.85	0.59
1:A:10:VAL:HG22	1:A:26:GLU:O	2.03	0.59
3:D:843:PHE:HE1	3:D:864:VAL:HG11	1.66	0.59
2:C:677:MET:HB3	2:C:987:ILE:HD13	1.84	0.59
2:C:1008:ARG:HH11	2:C:1028:GLY:HA2	1.68	0.59
3:D:462:GLN:HB2	3:D:513:ILE:HG21	1.83	0.59
3:D:808:THR:HG22	3:D:810:GLU:H	1.67	0.59
3:D:1012:GLU:HB2	3:D:1021:TYR:OH	2.03	0.59
2:M:92:ALA:HB2	2:M:120:LEU:HD11	1.85	0.59
3:N:994:GLN:NE2	3:N:998:GLU:OE2	2.36	0.59
3:N:1252:ILE:HG23	3:N:1253:THR:HG23	1.84	0.58
2:C:64:LEU:HD22	2:C:100:LEU:HD11	1.84	0.58
2:C:627:ARG:NH1	2:C:638:ASP:OD2	2.36	0.58
2:C:711:GLU:O	2:C:758:ARG:NH1	2.36	0.58
2:C:853:LEU:HB2	2:C:858:MET:CE	2.33	0.58
2:C:484:VAL:HG21	2:C:531:PHE:HE2	1.68	0.58
3:D:142:LEU:HG	3:D:143:ASN:H	1.66	0.58
3:D:248:PRO:HG3	3:D:308:LYS:HG3	1.85	0.58
3:N:1010:ASN:OD1	3:N:1014:ASN:ND2	2.35	0.58
3:N:1083:ASP:OD1	3:N:1087:ARG:CG	2.51	0.58
1:A:185:ARG:HB2	1:A:189:ARG:O	2.04	0.58
2:C:160:ALA:HB3	2:C:174:LEU:HB2	1.84	0.58
2:C:758:ARG:HE	2:C:788:THR:HB	1.68	0.58
3:N:1094:LEU:HD22	3:N:1260:ILE:HG12	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:1108:ARG:NH2	3:N:1198:TYR:O	2.36	0.58
3:N:1189:ARG:HB3	3:N:1204:CYS:HA	1.84	0.58
3:N:1290:LEU:HD12	3:N:1307:LYS:HA	1.83	0.58
1:K:83:LYS:HE3	1:K:168:ASP:HB2	1.84	0.58
3:N:14:SER:HB3	3:N:511:TRP:CE2	2.39	0.58
1:A:179:PHE:HB3	1:A:197:LEU:HD23	1.85	0.58
1:A:218:LEU:HD23	1:B:222:LEU:HD21	1.84	0.58
3:N:1045:MET:HE2	3:N:1073:SER:HA	1.86	0.58
2:M:660:ALA:HB1	2:M:667:ALA:O	2.04	0.58
2:C:267:TYR:CE2	2:C:290:LEU:HG	2.38	0.57
2:C:582:GLY:HA2	2:C:902:ILE:HD13	1.85	0.57
3:D:584:ASN:OD1	3:D:590:PRO:HD2	2.04	0.57
3:D:1190:SER:OG	3:D:1369:GLU:OE1	2.18	0.57
3:N:237:LYS:O	3:N:240:GLU:HB3	2.04	0.57
2:C:169:GLY:HA3	2:C:267:TYR:CD1	2.39	0.57
2:C:402:SER:HA	2:C:566:THR:HG23	1.85	0.57
2:C:736:ASP:O	2:C:744:ARG:HG2	2.04	0.57
3:D:244:GLU:HG3	3:D:310:LEU:HG	1.86	0.57
3:D:1108:ARG:NH2	3:D:1198:TYR:O	2.38	0.57
2:M:353:ARG:HH22	6:R:9:DG:H3'	1.69	0.57
3:D:356:PRO:HG2	3:D:359:ALA:HB2	1.86	0.57
2:M:775:ARG:HD3	2:M:782:ALA:HB2	1.86	0.57
3:N:1233:GLY:C	3:N:1235:GLN:N	2.60	0.57
5:P:404:ALA:O	5:P:408:LEU:HB2	2.03	0.57
5:P:411:HIS:O	5:P:415:THR:HB	2.03	0.57
3:D:63:TYR:OH	3:D:74:GLU:OE2	2.19	0.57
3:N:273:ARG:HB3	3:N:278:PRO:HA	1.85	0.57
1:A:70:GLY:HA3	1:A:136:GLY:HA3	1.86	0.57
3:D:192:ALA:HB3	3:D:195:VAL:HB	1.87	0.57
3:N:368:VAL:HB	3:N:377:VAL:HB	1.87	0.57
3:N:1083:ASP:OD1	3:N:1087:ARG:CZ	2.53	0.57
2:C:714:ASP:OD1	2:C:820:ARG:NH2	2.36	0.57
2:M:35:PRO:HG2	2:M:38:LYS:HD3	1.86	0.57
2:M:996:LYS:HE2	2:M:1000:MET:HE2	1.86	0.57
3:N:1143:GLY:O	3:N:1147:ARG:HD2	2.04	0.57
3:D:204:LEU:HD23	3:D:441:ARG:CZ	2.35	0.57
2:M:162:ILE:HB	2:M:172:ILE:HB	1.86	0.57
2:M:405:ARG:HD2	2:M:442:GLU:OE2	2.05	0.57
2:M:751:PRO:HB3	2:M:794:PRO:HA	1.86	0.57
3:N:1258:ARG:NH2	3:N:1351:GLU:HG2	2.13	0.57
2:C:420:ARG:NH1	2:C:420:ARG:HB2	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:580:MET:HE3	2:C:902:ILE:HG12	1.86	0.57
2:M:437:ARG:NH1	2:M:491:GLU:OE2	2.35	0.57
2:M:911:GLU:OE2	3:N:1062:ARG:NH1	2.38	0.57
2:M:1037:VAL:HG13	2:M:1049:LEU:HD11	1.86	0.57
4:O:40:LEU:HG	4:O:67:GLU:HG2	1.87	0.57
2:C:343:GLN:HG3	2:C:385:PHE:HB2	1.87	0.56
5:F:113:ILE:HD13	5:F:128:ARG:HG3	1.86	0.56
1:K:216:GLU:OE2	1:K:219:ARG:NH2	2.38	0.56
5:P:414:ARG:O	5:P:415:THR:C	2.48	0.56
1:A:74:ASP:OD1	1:A:76:VAL:HG12	2.05	0.56
2:C:272:ALA:HA	2:C:464:LEU:HD12	1.87	0.56
2:C:1115:LEU:HB3	3:D:85:VAL:HG12	1.87	0.56
5:P:79:ASP:O	5:P:79:ASP:CG	2.47	0.56
1:A:39:PRO:HG3	1:B:39:PRO:CG	2.35	0.56
5:F:131:VAL:HG13	5:F:178:ARG:HD3	1.87	0.56
1:K:133:GLU:HG2	1:K:134:GLU:H	1.70	0.56
2:M:684:PHE:HB3	3:N:633:VAL:HG21	1.86	0.56
2:M:1053:LEU:HA	3:N:621:LYS:HD2	1.87	0.56
7:Q:14:DG:H2'	7:Q:15:BRU:BR	2.61	0.56
2:C:261:ILE:HG23	2:C:290:LEU:HB2	1.88	0.56
3:D:1000:THR:HA	3:D:1041:LEU:HD11	1.88	0.56
1:B:32:PHE:HA	1:B:35:THR:HB	1.88	0.56
3:D:141:ILE:HG13	3:D:145:VAL:O	2.06	0.56
2:M:1103:ASP:HB3	2:M:1105:LYS:H	1.71	0.56
3:N:1101:VAL:HG21	3:N:1424:VAL:HB	1.87	0.56
3:D:584:ASN:CG	3:D:590:PRO:HD2	2.30	0.56
3:N:562:ALA:O	5:P:140:ARG:NH2	2.33	0.56
2:C:948:GLU:HB3	2:C:953:VAL:HG23	1.88	0.56
2:M:136:ILE:HB	2:M:336:VAL:HG12	1.86	0.56
3:D:814:ALA:O	3:D:818:ARG:HG3	2.05	0.56
5:F:368:VAL:HG22	5:F:397:ILE:HD11	1.87	0.56
1:K:50:GLY:HA3	1:K:171:PHE:O	2.06	0.56
1:B:58:ILE:HD12	1:B:140:MET:HE2	1.87	0.55
3:D:242:LEU:HD23	3:D:285:PRO:HG3	1.88	0.55
5:F:270:LYS:HG2	5:F:295:MET:HE1	1.87	0.55
2:M:1064:ASN:HA	5:P:341:PRO:HB3	1.88	0.55
3:N:56:TYR:HB3	3:N:65:ARG:O	2.05	0.55
2:C:944:LEU:HD22	2:C:962:GLN:HB3	1.88	0.55
3:D:1373:ARG:HG3	3:D:1374:GLN:N	2.20	0.55
2:M:628:PHE:H	2:M:638:ASP:CB	2.19	0.55
3:D:633:VAL:HG13	3:D:635:PRO:HD3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:759:ALA:HA	3:D:763:MET:HB2	1.88	0.55
1:K:201:THR:HG22	1:K:203:GLY:H	1.70	0.55
2:C:477:GLY:O	2:C:508:ILE:HG12	2.05	0.55
2:C:773:LEU:HD23	5:F:354:LEU:HD13	1.88	0.55
2:M:462:ASP:HB3	2:M:468:ARG:HD2	1.88	0.55
2:C:540:PHE:CE1	2:C:906:PHE:HE2	2.24	0.55
3:D:209:ARG:N	3:D:389:GLU:O	2.28	0.55
3:D:181:ASP:HB2	3:D:205:TYR:CD1	2.42	0.55
3:D:584:ASN:HD21	3:D:590:PRO:HD2	1.71	0.55
3:D:845:ASN:OD1	3:D:847:ASP:HB2	2.07	0.55
3:N:1198:TYR:OH	3:N:1432:LYS:NZ	2.35	0.55
3:N:1460:ILE:HG13	3:N:1461:GLY:H	1.72	0.55
5:P:79:ASP:OD1	5:P:81:VAL:HB	2.07	0.55
6:R:10:DA:H2"	6:R:11:DG:H5"	1.89	0.55
2:C:953:VAL:HB	2:C:962:GLN:HG2	1.87	0.55
3:D:959:GLU:HB3	3:D:963:TYR:HE1	1.71	0.55
5:P:416:ARG:C	5:P:417:LYS:HG2	2.32	0.55
1:B:112:ARG:HG3	1:B:113:ASP:OD1	2.07	0.55
1:K:206:THR:HB	1:K:209:GLU:HG3	1.89	0.55
1:B:30:ARG:NH2	2:C:854:PRO:HB3	2.22	0.55
2:C:290:LEU:HD22	2:C:302:VAL:HG11	1.89	0.55
2:M:580:MET:SD	2:M:584:GLU:HG3	2.45	0.55
3:N:45:PHE:HB3	3:N:86:ARG:HH22	1.71	0.55
2:C:399:ASN:ND2	2:C:568:ALA:O	2.37	0.55
2:C:689:VAL:HB	2:C:870:ILE:HD12	1.88	0.55
3:N:1083:ASP:O	3:N:1087:ARG:HG2	2.07	0.55
2:C:169:GLY:HA3	2:C:267:TYR:HD1	1.72	0.54
2:C:1053:LEU:HD11	3:D:1466:VAL:HG13	1.89	0.54
3:D:1277:ILE:HG22	3:D:1278:ASP:H	1.71	0.54
2:M:850:ALA:HA	3:N:632:VAL:CG2	2.38	0.54
2:M:911:GLU:HG3	2:M:912:PRO:HD3	1.90	0.54
1:A:219:ARG:HG3	1:A:220:GLU:N	2.22	0.54
2:C:135:VAL:HG23	2:C:395:LYS:HG3	1.89	0.54
2:C:983:ILE:HG21	2:C:987:ILE:HD11	1.89	0.54
3:D:237:LYS:N	3:D:240:GLU:OE1	2.35	0.54
3:D:1021:TYR:O	3:D:1025:GLN:HG2	2.07	0.54
2:M:690:ILE:HB	2:M:852:ILE:HD13	1.89	0.54
5:P:383:LEU:HD23	5:P:383:LEU:H	1.71	0.54
1:A:178:ALA:HB2	2:C:864:GLY:N	2.23	0.54
2:C:25:SER:OG	2:C:335:THR:OG1	2.12	0.54
3:D:1194:CYS:CB	3:D:1204:CYS:SG	2.80	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1275:SER:HA	3:D:1303:TYR:HE1	1.71	0.54
2:M:1102:LEU:HB2	3:N:7:LYS:HB2	1.89	0.54
3:N:1254:GLN:HB3	3:N:1258:ARG:HB2	1.89	0.54
2:C:787:ASP:OD1	2:C:789:SER:OG	2.26	0.54
2:C:889:HIS:O	2:C:892:LEU:HB3	2.07	0.54
3:D:1439:SER:HB2	3:D:1463:LYS:NZ	2.23	0.54
2:M:269:LEU:HB2	2:M:288:ARG:O	2.07	0.54
3:N:864:VAL:HG12	3:N:865:THR:H	1.71	0.54
3:N:952:ASP:HA	3:N:1062:ARG:HH21	1.72	0.54
7:Q:14:DG:H2'	7:Q:15:BRU:H6	1.89	0.54
3:N:890:VAL:O	3:N:926:LYS:NZ	2.38	0.54
2:C:504:GLU:HG2	2:C:509:ALA:HB2	1.88	0.54
3:D:1100:ASP:OD1	3:D:1463:LYS:NZ	2.30	0.54
1:K:206:THR:HG22	1:K:208:LEU:H	1.73	0.54
2:M:41:ASN:O	2:M:46:ALA:HB2	2.08	0.54
3:N:584:ASN:HD21	3:N:590:PRO:HD2	1.72	0.54
3:N:658:LEU:HA	3:N:661:MET:HE3	1.90	0.54
2:C:405:ARG:HD2	2:C:442:GLU:OE2	2.07	0.54
2:C:862:PRO:HB3	2:C:929:ARG:HH21	1.73	0.54
3:D:705:ALA:HA	3:D:706:PRO:C	2.33	0.54
3:N:154:THR:HG22	3:N:156:GLU:H	1.72	0.54
2:C:420:ARG:HB2	2:C:420:ARG:CZ	2.38	0.54
2:C:996:LYS:HE2	2:C:1000:MET:HE2	1.90	0.54
3:D:368:VAL:HB	3:D:377:VAL:HB	1.90	0.54
3:D:526:PRO:HB2	3:D:528:VAL:HG13	1.90	0.54
3:D:630:VAL:O	3:D:725:SER:HB2	2.07	0.54
3:D:760:ARG:NH2	4:E:3:GLU:OE1	2.26	0.54
4:E:3:GLU:O	4:E:6:ILE:HB	2.08	0.54
3:N:843:PHE:HB2	3:N:866:VAL:HG22	1.89	0.54
5:P:401:GLU:O	5:P:405:LEU:HB2	2.08	0.54
1:A:41:ARG:HG3	1:A:177:VAL:HG12	1.90	0.54
3:D:1258:ARG:HH21	3:D:1351:GLU:HG2	1.72	0.54
2:M:1009:SER:HB3	3:N:651:GLU:O	2.06	0.54
3:N:45:PHE:HD1	3:N:522:PRO:HB3	1.72	0.54
3:N:584:ASN:OD1	3:N:590:PRO:HD2	2.07	0.54
3:N:1233:GLY:O	3:N:1236:LEU:N	2.30	0.54
5:P:79:ASP:O	5:P:82:ARG:N	2.40	0.54
7:G:12:DG:H2'	7:G:13:DA:C8	2.42	0.54
2:C:675:ALA:HB2	2:C:867:VAL:HG11	1.89	0.53
2:M:144:PRO:HB2	2:M:273:GLY:HA3	1.90	0.53
2:M:1106:ASP:OD1	3:N:7:LYS:NZ	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:153:PRO:HA	5:F:156:VAL:HG22	1.91	0.53
2:M:470:PRO:HB2	2:M:534:VAL:HG21	1.90	0.53
1:A:70:GLY:N	2:C:607:ASP:OD1	2.36	0.53
2:C:768:THR:HG21	5:F:347:GLN:NE2	2.23	0.53
3:D:1225:ALA:HA	3:D:1367:HIS:ND1	2.24	0.53
3:N:26:VAL:HG11	3:N:44:LEU:HD23	1.91	0.53
5:P:408:LEU:C	5:P:412:GLU:HG2	2.33	0.53
1:A:18:ARG:O	1:A:207:PRO:HD3	2.09	0.53
2:C:154:ARG:HG3	2:C:177:GLU:OE2	2.09	0.53
3:D:1152:GLU:HG3	3:D:1162:GLU:HG3	1.89	0.53
3:D:1488:ASP:HA	4:E:73:LEU:HD23	1.90	0.53
3:N:171:LEU:HD22	3:N:390:PRO:HG2	1.91	0.53
3:N:1083:ASP:OD2	3:N:1087:ARG:NH1	2.41	0.53
3:N:1277:ILE:HG22	3:N:1278:ASP:H	1.73	0.53
3:N:1364:HIS:ND1	3:N:1366:LYS:HB2	2.24	0.53
3:D:486:ARG:H	3:D:486:ARG:HD2	1.72	0.53
3:D:739:ASP:OD1	3:D:741:ASP:OD1	2.27	0.53
2:M:409:ARG:HH22	2:M:442:GLU:HG2	1.74	0.53
2:M:1090:LYS:HD3	2:M:1112:PHE:CZ	2.43	0.53
3:N:1326:THR:HG22	3:N:1327:ARG:H	1.71	0.53
2:C:230:ARG:HG2	2:C:231:PRO:HD2	1.90	0.53
3:D:780:LYS:HE3	3:D:908:LYS:HE2	1.90	0.53
3:D:815:ALA:O	3:D:820:GLU:HB2	2.08	0.53
1:A:150:TYR:CE2	1:A:152:PRO:HG3	2.44	0.53
2:C:437:ARG:NH1	2:C:491:GLU:OE2	2.38	0.53
3:D:236:TYR:H	3:D:319:ALA:HB3	1.74	0.53
3:D:800:LYS:HB3	3:D:822:ALA:HB2	1.90	0.53
3:N:103:TRP:CE2	3:N:1444:THR:HG22	2.44	0.53
5:P:369:LEU:HD12	5:P:401:GLU:HB2	1.91	0.53
2:C:211:LEU:HD23	2:C:218:VAL:HG22	1.90	0.53
2:M:713:ARG:H	2:M:720:GLU:HB2	1.74	0.53
6:H:3:DT:H2"	6:H:4:DA:C8	2.44	0.53
3:D:87:ARG:HG2	3:D:523:ASP:HB3	1.90	0.53
5:F:365:GLU:HB2	5:F:404:ALA:HB2	1.89	0.53
3:N:260:GLU:HB3	3:N:271:VAL:HB	1.90	0.53
3:D:1168:MET:HE2	3:D:1172:HIS:CE1	2.43	0.53
5:P:411:HIS:C	5:P:415:THR:HB	2.33	0.53
1:A:91:ASN:O	1:A:94:LEU:HB3	2.09	0.52
2:C:198:ARG:NH2	2:C:203:ASP:OD2	2.42	0.52
3:N:204:LEU:HD23	3:N:441:ARG:CZ	2.39	0.52
3:N:1097:LYS:O	3:N:1101:VAL:HG23	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:LEU:O	1:A:174:VAL:HG21	2.09	0.52
3:D:788:GLY:HA3	3:D:938:GLY:O	2.10	0.52
3:D:1035:ILE:HA	3:D:1038:LEU:HD12	1.91	0.52
3:N:1127:GLU:HB2	3:N:1133:ARG:HB3	1.91	0.52
1:B:123:MET:O	1:B:125:PRO:HD3	2.09	0.52
2:C:582:GLY:N	2:C:584:GLU:OE2	2.42	0.52
3:D:50:PHE:CD2	3:D:522:PRO:HD3	2.44	0.52
3:D:231:VAL:O	3:D:236:TYR:OH	2.26	0.52
2:M:474:VAL:HG22	2:M:479:VAL:HG22	1.91	0.52
2:M:690:ILE:HG23	2:M:694:LEU:HD12	1.89	0.52
1:A:63:HIS:HD2	2:C:746:GLY:HA2	1.74	0.52
3:D:835:SER:H	3:D:838:ARG:HD2	1.74	0.52
1:K:178:ALA:HB2	2:M:864:GLY:N	2.25	0.52
2:M:248:PRO:C	2:M:250:ARG:H	2.17	0.52
2:M:249:LYS:C	2:M:251:ASP:H	2.17	0.52
2:M:283:ILE:HD13	2:M:305:PRO:HG2	1.92	0.52
3:D:1089:ALA:O	7:G:14:DG:H5''	2.08	0.52
1:L:205:VAL:HG12	1:L:206:THR:H	1.75	0.52
2:M:15:LEU:HD23	2:M:18:LEU:HD21	1.91	0.52
2:M:84:ARG:HA	2:M:131:GLY:HA2	1.90	0.52
5:P:396:ARG:NH2	5:P:400:ILE:HD12	2.24	0.52
2:C:128:ILE:O	2:C:129:ILE:HD13	2.10	0.52
3:D:1047:LYS:HG2	3:D:1053:PHE:CE1	2.45	0.52
3:D:1149:LEU:HD21	3:D:1166:LEU:HD21	1.92	0.52
3:N:90:MET:HE3	3:N:521:PRO:HD3	1.92	0.52
2:C:331:ARG:NH2	2:C:427:VAL:HG12	2.25	0.52
2:C:751:PRO:HB3	2:C:794:PRO:HA	1.92	0.52
3:D:254:GLU:O	3:D:300:LYS:HG3	2.09	0.52
3:D:803:GLY:HA2	3:D:826:PRO:O	2.10	0.52
3:N:759:ALA:HA	3:N:763:MET:HB2	1.92	0.52
5:P:394:ARG:HG2	5:P:395:GLU:HG2	1.90	0.52
1:B:57:TYR:CE1	1:B:163:ASN:HB2	2.40	0.52
2:C:502:PRO:HG2	2:C:510:ALA:HB2	1.92	0.52
3:D:689:ASP:HB3	4:E:51:LEU:HD11	1.91	0.52
3:D:1395:LEU:HD11	3:D:1400:VAL:HB	1.90	0.52
5:F:397:ILE:HA	5:F:400:ILE:HG12	1.92	0.52
2:M:208:ALA:HB2	2:M:222:MET:HE1	1.91	0.52
3:N:996:TRP:CD2	3:N:1056:PRO:HG3	2.44	0.52
3:D:879:ARG:O	3:D:902:LEU:HD11	2.09	0.52
2:M:879:ARG:HD2	2:M:879:ARG:N	2.24	0.52
3:N:576:GLU:OE2	3:N:587:ARG:NH1	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:83:LYS:NZ	3:D:842:VAL:O	2.43	0.51
2:C:92:ALA:HB2	2:C:120:LEU:HD11	1.91	0.51
3:D:42:ASP:OD1	3:D:48:ARG:NH2	2.43	0.51
3:D:236:TYR:HB3	3:D:313:MET:HG3	1.91	0.51
5:F:95:THR:HG22	5:F:96:LEU:H	1.75	0.51
1:K:215:VAL:HG12	1:L:222:LEU:HD22	1.91	0.51
3:N:137:PRO:HB3	3:N:147:VAL:HG12	1.90	0.51
3:N:520:LEU:HD12	3:N:521:PRO:HD2	1.92	0.51
2:C:214:TYR:O	2:C:218:VAL:HG23	2.10	0.51
2:C:437:ARG:CZ	2:C:488:ALA:HA	2.39	0.51
2:C:874:LEU:HD22	3:D:1029:ARG:HB2	1.92	0.51
3:D:1097:LYS:O	3:D:1101:VAL:HG23	2.10	0.51
3:N:869:MET:HE3	3:N:894:LYS:HE3	1.92	0.51
3:N:1083:ASP:CG	3:N:1087:ARG:NH1	2.69	0.51
2:C:262:ALA:HA	2:C:289:THR:CG2	2.41	0.51
1:L:57:TYR:HE1	1:L:163:ASN:HB2	1.75	0.51
2:M:32:ALA:HB2	2:M:73:LEU:HD12	1.91	0.51
3:N:539:ASP:OD1	5:P:316:SER:OG	2.27	0.51
5:P:125:ASP:OD1	5:P:125:ASP:N	2.27	0.51
2:C:1060:ILE:HD11	2:C:1083:GLU:HG2	1.93	0.51
3:D:1117:TYR:HA	3:D:1193:THR:HG21	1.93	0.51
1:L:124:ASN:OD1	1:L:124:ASN:N	2.43	0.51
2:M:89:THR:OG1	2:M:129:ILE:O	2.27	0.51
3:N:132:TYR:HB2	3:N:153:LEU:HD12	1.91	0.51
3:N:534:ARG:HH12	5:P:312:GLN:HB3	1.76	0.51
3:D:1103:HIS:HA	3:D:1223:ILE:HD11	1.93	0.51
5:F:218:GLN:O	5:F:222:ARG:HG2	2.10	0.51
3:N:314:PRO:HG2	3:N:317:VAL:CG1	2.40	0.51
2:C:198:ARG:NH2	2:C:228:ALA:O	2.44	0.51
3:D:27:GLU:O	3:D:552:ASN:ND2	2.43	0.51
1:L:56:VAL:HG13	1:L:142:VAL:HG12	1.92	0.51
2:M:607:ASP:HB2	2:M:610:ARG:NH1	2.26	0.51
2:M:675:ALA:HB2	2:M:867:VAL:HG11	1.93	0.51
3:N:181:ASP:HB2	3:N:205:TYR:CD1	2.45	0.51
3:N:355:VAL:HG11	3:N:385:VAL:HG21	1.93	0.51
3:N:483:HIS:CD2	3:N:485:SER:H	2.29	0.51
5:P:360:LYS:NZ	5:P:416:ARG:HD3	2.25	0.51
2:C:942:GLU:OE2	2:C:945:ARG:NH2	2.37	0.51
5:F:361:LEU:HB3	5:F:365:GLU:HG3	1.93	0.51
2:M:376:ARG:NH2	5:P:279:GLN:OE1	2.43	0.51
4:O:32:ARG:O	4:O:95:VAL:HG21	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:389:SER:OG	2:C:390:GLN:N	2.43	0.51
3:N:192:ALA:HB3	3:N:195:VAL:HB	1.92	0.51
1:A:61:VAL:HG21	1:A:75:VAL:HG21	1.93	0.51
1:L:213:GLN:O	1:L:217:ILE:HG13	2.11	0.51
2:M:355:VAL:HG13	2:M:372:LEU:HG	1.92	0.51
3:N:584:ASN:ND2	3:N:590:PRO:HD2	2.25	0.51
4:O:95:VAL:O	4:O:95:VAL:HG12	2.11	0.51
2:C:256:TYR:HE1	6:H:10:DA:H61	1.57	0.51
3:D:134:VAL:HG22	3:D:151:GLN:O	2.11	0.51
3:D:475:LYS:HA	3:D:478:LEU:HD12	1.92	0.51
3:D:543:LEU:O	3:D:546:ARG:HG2	2.11	0.51
3:D:583:ASP:CG	3:D:586:ARG:HG3	2.35	0.51
3:D:683:ILE:HG21	3:D:688:TRP:CZ2	2.46	0.51
2:M:326:ASP:OD1	6:R:14:DG:N2	2.34	0.51
2:M:487:THR:HG23	2:M:490:GLU:H	1.75	0.51
2:M:677:MET:HB3	2:M:987:ILE:HD13	1.93	0.51
3:N:693:GLU:HA	4:O:48:MET:HE1	1.92	0.51
3:D:569:ASN:O	3:D:573:MET:HG3	2.11	0.50
2:M:768:THR:HB	2:M:771:GLU:HB2	1.92	0.50
3:N:1083:ASP:O	3:N:1087:ARG:HG3	2.11	0.50
1:B:80:LEU:HB3	3:D:867:ARG:NH2	2.27	0.50
3:D:256:GLU:OE2	3:D:300:LYS:HE3	2.12	0.50
2:M:853:LEU:HB2	2:M:858:MET:CE	2.37	0.50
2:M:1094:ALA:HA	3:N:518:PRO:HB2	1.92	0.50
1:A:193:ASP:HB3	2:C:938:LYS:HD2	1.92	0.50
2:C:139:GLN:HB2	2:C:391:LEU:HD11	1.92	0.50
3:D:1461:GLY:O	3:D:1465:ASN:ND2	2.32	0.50
4:E:17:TYR:O	4:E:21:VAL:HG23	2.11	0.50
2:M:358:ARG:HH12	2:M:374:ASN:HB2	1.75	0.50
2:M:1090:LYS:HE2	3:N:88:TYR:O	2.12	0.50
3:N:1124:GLN:HG3	3:N:1127:GLU:CD	2.37	0.50
2:C:6:PHE:CD2	2:C:909:ALA:HB2	2.46	0.50
3:D:702:LEU:O	3:D:713:ILE:HA	2.12	0.50
2:M:561:GLY:O	2:M:565:GLN:HG3	2.11	0.50
1:B:48:ILE:HD11	1:B:214:ALA:HB2	1.92	0.50
3:D:322:VAL:HG22	3:D:335:LEU:HD11	1.94	0.50
3:D:1156:LEU:HD23	3:D:1182:GLU:OE2	2.12	0.50
1:K:43:ILE:HG12	1:L:32:PHE:CZ	2.47	0.50
1:L:91:ASN:HB3	1:L:94:LEU:HB2	1.94	0.50
2:M:267:TYR:CE2	2:M:290:LEU:HG	2.45	0.50
5:P:411:HIS:C	5:P:412:GLU:OE1	2.55	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:236:ILE:HG23	2:C:248:PRO:HB3	1.94	0.50
2:C:244:PRO:HD2	5:F:82:ARG:NH1	2.26	0.50
2:C:290:LEU:HB3	2:C:303:PHE:HE1	1.77	0.50
2:C:340:MET:HE2	2:C:344:PHE:HB2	1.94	0.50
3:D:56:TYR:HB3	3:D:65:ARG:O	2.11	0.50
3:D:520:LEU:HD12	3:D:521:PRO:HD2	1.93	0.50
4:E:19:LEU:O	4:E:23:VAL:HG23	2.12	0.50
4:E:46:PRO:HB2	4:E:57:ASP:HB3	1.93	0.50
1:K:58:ILE:HB	1:K:61:VAL:HB	1.92	0.50
3:N:275:GLU:HG2	3:N:276:ASP:H	1.76	0.50
3:N:814:ALA:O	3:N:818:ARG:HG3	2.10	0.50
4:O:88:GLU:OE2	4:O:91:ARG:NH1	2.37	0.50
3:D:317:VAL:HG23	3:D:339:TRP:HB3	1.94	0.50
3:D:808:THR:HG22	3:D:810:GLU:N	2.27	0.50
3:D:843:PHE:CE1	3:D:864:VAL:HG11	2.45	0.50
2:M:910:LYS:HB3	2:M:912:PRO:HD2	1.93	0.50
3:N:705:ALA:HA	3:N:706:PRO:C	2.37	0.50
6:H:10:DA:H2''	6:H:11:DG:O4'	2.12	0.50
1:B:80:LEU:HD11	3:D:842:VAL:HG12	1.94	0.50
3:D:1161:GLU:CD	3:D:1164:ARG:HB2	2.36	0.50
5:F:364:ARG:O	5:F:368:VAL:HG23	2.11	0.50
1:K:4:SER:HA	1:K:189:ARG:HH12	1.77	0.50
1:L:5:LYS:HE3	1:L:6:LEU:H	1.77	0.50
3:N:1238:MET:O	3:N:1246:VAL:O	2.29	0.50
1:A:25:LEU:HD23	1:A:28:LEU:HD11	1.93	0.50
2:C:430:VAL:HG12	3:D:1075:HIS:CE1	2.47	0.50
2:C:644:VAL:HG22	2:C:645:VAL:H	1.76	0.50
2:C:1059:ASP:OD1	2:C:1080:SER:OG	2.25	0.50
3:D:890:VAL:HB	3:D:922:LEU:HD22	1.93	0.50
2:M:1051:GLU:HB3	2:M:1056:LYS:HE3	1.93	0.50
2:C:808:ARG:NH1	5:F:305:GLU:OE2	2.43	0.49
2:C:874:LEU:HD13	3:D:783:ARG:HB3	1.92	0.49
2:C:987:ILE:HA	3:D:948:THR:HG21	1.94	0.49
2:M:874:LEU:HD13	3:N:783:ARG:HB3	1.94	0.49
3:D:477:LEU:O	3:D:481:MET:HG2	2.12	0.49
3:D:1236:LEU:HB2	3:D:1256:LEU:HB2	1.94	0.49
3:N:633:VAL:C	3:N:635:PRO:HD3	2.37	0.49
3:D:142:LEU:HG	3:D:143:ASN:N	2.27	0.49
3:D:1462:LEU:O	3:D:1466:VAL:HG23	2.13	0.49
5:F:88:ILE:HD11	5:F:192:LEU:HD13	1.93	0.49
1:B:79:ILE:HA	1:B:82:LEU:HD12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:545:ASN:HB3	2:C:583:LEU:HD22	1.94	0.49
3:D:339:TRP:CZ3	3:D:341:GLU:HB2	2.46	0.49
3:N:801:GLY:O	3:N:804:LEU:HG	2.12	0.49
5:P:79:ASP:O	5:P:79:ASP:OD1	2.30	0.49
5:P:414:ARG:HG2	5:P:415:THR:N	2.19	0.49
3:D:15:PRO:O	3:D:19:ARG:HG3	2.13	0.49
3:N:42:ASP:N	3:N:46:ASP:OD2	2.39	0.49
3:N:890:VAL:HG23	3:N:892:ASP:H	1.77	0.49
3:D:270:LEU:HD12	3:D:284:LEU:HD11	1.95	0.49
3:D:806:PHE:O	3:D:829:VAL:HA	2.13	0.49
3:D:1066:THR:H	3:D:1069:GLU:HB2	1.78	0.49
3:D:1118:ILE:HD12	3:D:1192:LEU:HD12	1.95	0.49
3:D:1267:ARG:HG2	3:D:1331:ASP:OD1	2.12	0.49
2:M:121:MET:HE1	2:M:336:VAL:HG21	1.94	0.49
1:B:176:ARG:NH2	3:D:888:GLU:OE1	2.46	0.49
2:C:580:MET:SD	2:C:584:GLU:HG3	2.53	0.49
3:D:47:GLU:HA	3:D:51:GLY:O	2.12	0.49
3:D:1101:VAL:HG21	3:D:1424:VAL:HB	1.95	0.49
2:M:157:ARG:NH1	2:M:177:GLU:HG3	2.27	0.49
1:B:115:LEU:O	1:B:117:VAL:HG23	2.13	0.49
3:D:1208:ASP:OD1	3:D:1210:SER:OG	2.29	0.49
2:M:170:PRO:HA	6:R:13:DT:O4	2.13	0.49
2:M:343:GLN:HG3	2:M:385:PHE:HB2	1.95	0.49
2:M:358:ARG:HH22	2:M:374:ASN:HB2	1.78	0.49
1:A:56:VAL:HG23	1:A:167:VAL:HG21	1.95	0.49
2:C:425:PHE:CD1	3:D:1079:LYS:HG3	2.46	0.49
2:C:672:VAL:CG2	2:C:994:ILE:HD12	2.42	0.49
5:F:212:LEU:HD22	5:F:247:ILE:HG23	1.94	0.49
1:L:32:PHE:HA	1:L:35:THR:HB	1.94	0.49
2:M:777:ILE:O	5:P:409:LYS:HG3	2.12	0.49
3:N:15:PRO:O	3:N:19:ARG:HG3	2.13	0.49
3:N:236:TYR:HB2	3:N:319:ALA:HB3	1.95	0.49
3:N:850:LEU:HD12	3:N:884:ARG:NH2	2.27	0.49
2:C:98:LEU:HD12	2:C:113:VAL:HG21	1.95	0.48
2:C:413:LEU:HD12	2:C:452:ILE:HD11	1.94	0.48
3:D:1310:ARG:HD3	3:D:1327:ARG:HH11	1.78	0.48
2:M:422:ARG:NH2	6:R:14:DG:OP1	2.35	0.48
2:M:520:GLU:HG3	2:M:521:PRO:HD2	1.94	0.48
5:P:358:LEU:HD23	5:P:370:LYS:HE2	1.95	0.48
7:Q:15:BRU:C2	7:Q:16:DC:C5	2.96	0.48
1:B:20:TYR:C	1:B:207:PRO:HG2	2.39	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:102:LYS:HA	1:B:138:LEU:O	2.13	0.48
3:D:67:ARG:HH11	5:F:379:ARG:HB2	1.79	0.48
3:D:185:VAL:N	3:D:201:GLY:O	2.35	0.48
5:F:162:LYS:HE3	5:F:162:LYS:HB2	1.71	0.48
2:M:428:ARG:NH2	2:M:447:ALA:O	2.45	0.48
3:N:584:ASN:OD1	3:N:585:GLY:N	2.46	0.48
1:A:111:ALA:O	1:A:114:PHE:HD1	1.96	0.48
2:C:1089:VAL:HG13	2:C:1099:VAL:HB	1.96	0.48
5:F:110:MET:HA	5:F:113:ILE:HD12	1.96	0.48
5:F:363:GLU:O	5:F:367:MET:HB2	2.13	0.48
2:M:197:LEU:O	2:M:202:TYR:HB2	2.12	0.48
3:N:405:ASP:CG	3:N:406:ASP:H	2.21	0.48
3:N:1283:ILE:HG13	3:N:1315:ASP:HB3	1.94	0.48
1:B:65:PHE:HE1	3:D:809:PRO:HG2	1.77	0.48
2:C:397:GLU:HB3	2:C:403:SER:HB3	1.94	0.48
2:C:540:PHE:HB3	2:C:544:THR:HB	1.96	0.48
2:C:1059:ASP:OD2	2:C:1062:GLY:HA3	2.13	0.48
3:D:46:ASP:HB3	3:D:49:ILE:HG13	1.95	0.48
3:D:1003:VAL:HG21	3:D:1041:LEU:HG	1.95	0.48
2:M:607:ASP:HB3	2:M:610:ARG:H	1.79	0.48
3:N:853:VAL:HG22	3:N:858:VAL:HG23	1.96	0.48
3:N:1380:GLU:HB2	3:N:1420:LEU:HD22	1.95	0.48
5:P:411:HIS:O	5:P:412:GLU:OE1	2.30	0.48
2:C:258:TYR:CE2	2:C:293:PHE:HB2	2.49	0.48
3:D:828:LYS:HA	3:D:832:ARG:HA	1.94	0.48
2:M:957:LYS:HG2	2:M:961:GLU:OE1	2.13	0.48
3:N:187:LYS:HG3	3:N:198:ARG:O	2.13	0.48
2:C:184:MET:HE2	2:C:191:PHE:HE2	1.77	0.48
3:D:171:LEU:HD11	3:D:192:ALA:HB2	1.94	0.48
3:D:770:LEU:HB2	3:D:1210:SER:HA	1.95	0.48
4:E:37:ASN:OD1	4:E:37:ASN:N	2.38	0.48
1:A:202:ASP:OD1	1:A:204:SER:OG	2.22	0.48
2:C:20:GLU:HG3	2:C:21:ILE:N	2.28	0.48
2:C:1009:SER:HB3	3:D:651:GLU:O	2.14	0.48
2:M:286:SER:OG	2:M:301:GLU:OE2	2.18	0.48
2:M:456:ALA:HB3	2:M:459:ALA:HB2	1.96	0.48
2:M:1054:THR:HG22	2:M:1082:PRO:HG3	1.94	0.48
3:N:959:GLU:HB3	3:N:963:TYR:CE1	2.49	0.48
5:P:79:ASP:O	5:P:80:PRO:C	2.57	0.48
2:C:700:TYR:HD2	2:C:996:LYS:HB2	1.78	0.48
3:D:58:CYS:HB2	3:D:76:CYS:SG	2.53	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:927:THR:O	3:D:931:LEU:HG	2.13	0.48
1:L:20:TYR:C	1:L:207:PRO:HG2	2.38	0.48
2:M:30:LEU:O	2:M:71:TYR:OH	2.29	0.48
2:M:976:ASP:CG	2:M:978:ARG:HH11	2.22	0.48
2:C:102:HIS:HB3	2:C:105:THR:HB	1.95	0.48
2:C:221:LEU:HD11	2:C:307:LEU:HD21	1.95	0.48
3:D:573:MET:SD	5:F:210:LEU:HB3	2.54	0.48
3:D:1045:MET:HE2	3:D:1073:SER:HA	1.95	0.48
2:M:292:ARG:O	2:M:298:PHE:HD2	1.96	0.48
2:M:943:VAL:HG21	2:M:973:VAL:HG13	1.96	0.48
3:N:143:ASN:OD1	3:N:144:GLY:N	2.45	0.48
3:N:675:ARG:HH12	5:P:420:ASP:HB3	1.78	0.48
5:P:413:SER:O	5:P:417:LYS:O	2.32	0.48
1:B:161:ARG:HE	1:B:161:ARG:HB2	1.44	0.48
2:C:577:PRO:HG2	2:C:580:MET:HG2	1.96	0.48
3:D:171:LEU:HD12	3:D:195:VAL:HG21	1.95	0.48
3:D:1211:MET:HB3	3:D:1213:ARG:HE	1.77	0.48
5:P:367:MET:O	5:P:371:LEU:HG	2.13	0.48
1:B:56:VAL:HG13	1:B:142:VAL:HG12	1.96	0.47
1:B:91:ASN:HB3	1:B:94:LEU:HB2	1.96	0.47
2:C:182:VAL:HG23	2:C:193:LEU:HB3	1.94	0.47
2:C:260:LEU:C	2:C:261:ILE:HD12	2.39	0.47
2:C:1060:ILE:O	2:C:1063:ARG:HG2	2.14	0.47
2:M:504:GLU:HG2	2:M:509:ALA:HB2	1.96	0.47
2:M:627:ARG:HA	2:M:638:ASP:HB2	1.96	0.47
2:M:1031:ARG:NE	7:Q:16:DC:OP1	2.46	0.47
2:M:1054:THR:O	2:M:1059:ASP:HB3	2.14	0.47
5:P:79:ASP:CG	6:R:8:DG:H1	2.20	0.47
2:C:385:PHE:O	2:C:389:SER:HB3	2.14	0.47
3:D:1211:MET:SD	4:E:16:LYS:HD3	2.54	0.47
3:N:1194:CYS:O	3:N:1373:ARG:NH2	2.46	0.47
5:P:371:LEU:HD23	5:P:376:ILE:HD11	1.96	0.47
2:C:300:ASP:OD1	2:C:301:GLU:N	2.47	0.47
2:C:965:GLU:O	2:C:969:GLN:HG3	2.14	0.47
3:D:636:GLN:NE2	3:D:727:GLN:OE1	2.48	0.47
1:A:57:TYR:CE1	1:A:161:ARG:HD2	2.49	0.47
1:B:227:ASN:HA	1:B:228:PRO:HD3	1.66	0.47
2:C:243:ARG:NH2	6:H:9:DG:O6	2.45	0.47
2:C:357:GLU:O	2:C:361:MET:HE2	2.14	0.47
2:C:489:THR:O	2:C:492:ASP:HB2	2.14	0.47
2:C:682:TYR:CD1	2:C:851:LYS:HB2	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:834:GLN:O	2:C:837:ASP:HB2	2.14	0.47
2:M:439:CYS:HB2	2:M:541:SER:HB3	1.96	0.47
2:M:911:GLU:O	2:M:915:LYS:HG2	2.13	0.47
3:N:1272:ALA:HA	3:N:1326:THR:HB	1.96	0.47
4:E:57:ASP:O	4:E:63:TRP:NE1	2.38	0.47
5:F:268:ILE:HD13	5:F:311:ALA:HB2	1.96	0.47
2:M:540:PHE:HB3	2:M:544:THR:HB	1.94	0.47
3:N:1044:LEU:HD12	3:N:1044:LEU:H	1.78	0.47
2:C:249:LYS:C	2:C:251:ASP:H	2.23	0.47
2:C:607:ASP:HB2	2:C:610:ARG:NH1	2.29	0.47
2:C:1056:LYS:O	3:D:624:ASP:N	2.47	0.47
2:C:1071:ILE:HG23	3:D:670:VAL:HG21	1.96	0.47
3:D:251:PHE:HZ	3:D:282:TYR:CD1	2.32	0.47
3:D:1390:LEU:O	3:D:1393:GLN:HG2	2.15	0.47
1:K:8:ALA:HA	1:K:9:PRO:HD3	1.63	0.47
2:M:182:VAL:HG23	2:M:193:LEU:HB3	1.97	0.47
2:M:385:PHE:O	2:M:389:SER:HB3	2.13	0.47
3:N:187:LYS:N	3:N:200:ASP:HB3	2.30	0.47
3:N:1156:LEU:HD23	3:N:1182:GLU:OE2	2.14	0.47
3:N:1236:LEU:CD1	3:N:1355:VAL:CG1	2.93	0.47
2:C:503:LEU:HD11	2:C:532:MET:HE1	1.97	0.47
2:C:692:GLU:O	2:C:696:LYS:HG3	2.14	0.47
3:D:554:LEU:HD23	3:D:574:LEU:HD22	1.97	0.47
3:D:760:ARG:NH1	4:E:59:ASN:OD1	2.47	0.47
3:D:1101:VAL:HB	3:D:1102:THR:HG23	1.96	0.47
3:D:1326:THR:HG22	3:D:1327:ARG:H	1.80	0.47
3:D:1486:VAL:CG2	4:E:22:VAL:HG13	2.45	0.47
3:N:1086:LEU:O	3:N:1088:THR:N	2.48	0.47
3:N:1101:VAL:HG22	3:N:1428:ALA:HB2	1.97	0.47
5:P:79:ASP:C	5:P:79:ASP:OD1	2.57	0.47
1:A:206:THR:HG22	1:A:209:GLU:H	1.80	0.47
2:C:586:ARG:O	2:C:586:ARG:HG3	2.15	0.47
3:D:479:GLU:OE1	3:D:482:LYS:NZ	2.48	0.47
3:D:642:CYS:HB3	3:D:716:PHE:CD1	2.50	0.47
2:M:169:GLY:HA3	2:M:267:TYR:CD1	2.50	0.47
3:N:1384:PRO:HB3	3:N:1389:LEU:O	2.15	0.47
1:A:13:VAL:HG13	1:A:23:PHE:CE1	2.50	0.47
2:C:41:ASN:O	2:C:46:ALA:HB2	2.15	0.47
2:C:286:SER:OG	2:C:301:GLU:OE2	2.31	0.47
2:C:578:VAL:HG23	2:C:579:VAL:HG23	1.96	0.47
2:C:1058:ASP:OD2	2:C:1084:SER:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:170:PRO:HA	3:D:392:SER:HB3	1.97	0.47
3:D:1440:PHE:O	3:D:1441:GLN:HG3	2.15	0.47
5:F:181:GLU:O	5:F:185:GLN:HG2	2.15	0.47
1:L:18:ARG:O	1:L:207:PRO:HD3	2.14	0.47
2:M:205:GLU:O	2:M:209:ARG:HG2	2.15	0.47
2:M:944:LEU:HD22	2:M:962:GLN:HB3	1.96	0.47
3:N:1086:LEU:C	3:N:1088:THR:N	2.71	0.47
1:B:64:GLU:HG2	1:B:75:VAL:CG1	2.45	0.47
1:B:216:GLU:OE2	1:B:219:ARG:NH2	2.35	0.47
2:C:248:PRO:C	2:C:250:ARG:H	2.23	0.47
2:C:726:ILE:HD11	2:C:757:GLY:HA3	1.97	0.47
2:C:892:LEU:O	2:C:895:TYR:HB3	2.15	0.47
2:M:1116:ALA:HB2	3:N:88:TYR:HB3	1.97	0.47
3:N:640:HIS:ND1	3:N:641:GLN:HG3	2.29	0.47
3:N:1238:MET:O	3:N:1246:VAL:C	2.58	0.47
2:C:258:TYR:HE2	2:C:293:PHE:HB2	1.79	0.46
2:C:471:TYR:CE2	2:C:496:ILE:HG21	2.50	0.46
2:C:480:THR:HB	2:C:482:GLU:HG2	1.97	0.46
3:D:373:PRO:O	3:D:376:GLU:HG2	2.15	0.46
2:M:594:ALA:HB1	2:M:654:LEU:HD11	1.97	0.46
3:N:1481:VAL:HB	4:O:18:ARG:HA	1.96	0.46
2:C:673:LEU:HD22	2:C:895:TYR:CE1	2.50	0.46
3:D:601:ARG:NH1	3:D:606:ILE:HG12	2.30	0.46
2:M:740:GLU:HB3	2:M:805:ARG:HH12	1.80	0.46
3:N:1404:ASN:HD21	3:N:1415:VAL:HG23	1.80	0.46
2:C:26:TYR:CE2	2:C:30:LEU:HD11	2.50	0.46
2:C:140:ILE:HD11	2:C:331:ARG:NE	2.30	0.46
2:C:437:ARG:NH2	2:C:488:ALA:HA	2.30	0.46
3:D:68:PHE:HB2	3:D:80:VAL:HG21	1.98	0.46
3:D:959:GLU:O	3:D:963:TYR:HD1	1.98	0.46
4:E:37:ASN:HB3	4:E:93:TYR:CD1	2.50	0.46
3:N:90:MET:HE2	3:N:90:MET:HB3	1.83	0.46
3:N:1282:ARG:HB3	3:N:1293:PHE:HB2	1.97	0.46
5:P:364:ARG:HG2	5:P:390:PHE:CE2	2.50	0.46
2:C:283:ILE:HG21	2:C:305:PRO:CG	2.46	0.46
3:D:17:LYS:O	3:D:20:SER:HB3	2.15	0.46
3:D:135:LEU:O	3:D:149:LYS:HG3	2.16	0.46
3:D:1189:ARG:HB3	3:D:1204:CYS:HA	1.98	0.46
1:L:24:VAL:HG11	1:L:194:LYS:HE3	1.97	0.46
2:M:480:THR:HB	2:M:482:GLU:HG2	1.96	0.46
2:M:930:LYS:HD2	2:M:930:LYS:HA	1.67	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:TYR:OH	2:C:832:LYS:HE2	2.15	0.46
1:A:191:ASP:OD1	1:A:191:ASP:N	2.36	0.46
2:C:680:ASP:H	3:D:943:THR:HB	1.80	0.46
2:C:987:ILE:HG23	3:D:948:THR:HB	1.97	0.46
2:C:1090:LYS:HD2	2:C:1090:LYS:HA	1.75	0.46
3:D:18:ILE:HG23	3:D:518:PRO:HG3	1.97	0.46
3:D:134:VAL:HG13	3:D:153:LEU:HD21	1.97	0.46
3:D:1008:PHE:O	3:D:1012:GLU:HB3	2.15	0.46
4:E:33:HIS:HB2	4:E:37:ASN:OD1	2.16	0.46
3:N:288:MET:HE2	3:N:307:ALA:HB2	1.97	0.46
3:N:843:PHE:CE1	3:N:864:VAL:HG11	2.51	0.46
5:P:358:LEU:O	5:P:366:ALA:HB2	2.16	0.46
1:A:70:GLY:HA3	1:A:136:GLY:CA	2.45	0.46
2:C:170:PRO:HA	6:H:13:DT:O4	2.16	0.46
2:C:281:LEU:HD22	2:C:306:THR:HA	1.98	0.46
3:D:19:ARG:HA	3:D:22:SER:HB3	1.98	0.46
3:N:136:ASP:H	3:N:453:ASP:HB3	1.80	0.46
4:O:48:MET:N	4:O:55:PHE:O	2.47	0.46
5:P:79:ASP:C	5:P:81:VAL:N	2.71	0.46
5:P:358:LEU:HD12	5:P:358:LEU:HA	1.78	0.46
1:A:101:LEU:HD21	1:A:109:VAL:HG11	1.97	0.46
1:A:191:ASP:O	2:C:938:LYS:NZ	2.49	0.46
2:C:295:ASP:N	2:C:295:ASP:OD1	2.49	0.46
2:C:1015:LEU:HD23	5:F:335:ASP:HA	1.97	0.46
2:C:1040:LEU:HD23	2:C:1040:LEU:HA	1.60	0.46
3:D:171:LEU:HD22	3:D:390:PRO:HG2	1.97	0.46
3:D:700:VAL:O	3:D:715:ALA:HA	2.15	0.46
3:D:911:LEU:O	3:D:915:VAL:HG23	2.16	0.46
3:D:1053:PHE:CE1	3:D:1072:ILE:HG23	2.50	0.46
3:D:1450:ALA:HA	3:D:1455:LYS:HD2	1.97	0.46
2:M:774:LEU:HD12	2:M:777:ILE:HD12	1.98	0.46
5:P:79:ASP:CG	5:P:82:ARG:H	2.22	0.46
1:B:37:GLY:HA3	1:B:179:PHE:CE1	2.50	0.46
2:C:500:ASN:OD1	3:D:1067:VAL:HG12	2.15	0.46
2:C:581:THR:N	2:C:584:GLU:OE2	2.49	0.46
2:C:630:ARG:HB2	2:C:705:ILE:HB	1.97	0.46
2:C:1088:LEU:HD13	3:D:613:ARG:HG2	1.98	0.46
1:K:183:ASP:HA	2:M:938:LYS:HE3	1.98	0.46
2:M:874:LEU:HD23	3:N:1023:MET:SD	2.55	0.46
3:N:1276:GLU:OE2	3:N:1301:LYS:HE2	2.16	0.46
2:C:235:LEU:HD21	2:C:254:VAL:HG22	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:685:GLU:HA	2:C:685:GLU:OE1	2.16	0.46
2:C:699:PHE:HB3	2:C:700:TYR:HD1	1.81	0.46
3:D:689:ASP:CB	4:E:51:LEU:HD11	2.46	0.46
3:D:964:LEU:HD23	3:D:964:LEU:HA	1.77	0.46
2:M:580:MET:HB3	2:M:584:GLU:CD	2.41	0.46
3:N:114:THR:HG23	3:N:495:ARG:HG2	1.98	0.46
3:N:963:TYR:CE2	3:N:1002:LYS:HD3	2.51	0.46
3:N:1047:LYS:HG2	3:N:1053:PHE:CZ	2.51	0.46
3:N:1236:LEU:HD13	3:N:1355:VAL:CG1	2.46	0.46
4:O:14:ASP:OD1	4:O:18:ARG:NH1	2.49	0.46
3:D:178:LEU:HD12	3:D:190:GLU:HB3	1.97	0.46
3:N:661:MET:HE1	3:N:677:LEU:HD11	1.97	0.46
1:A:31:GLY:O	1:B:42:ARG:NH2	2.45	0.45
2:C:194:VAL:HG13	2:C:221:LEU:HD23	1.97	0.45
2:C:280:LYS:HZ3	2:C:323:ASP:CG	2.24	0.45
3:D:351:MET:HB3	3:D:370:ALA:HB2	1.98	0.45
3:D:849:ALA:O	3:D:853:VAL:HG23	2.15	0.45
3:D:1122:LEU:HD11	3:D:1186:VAL:HG23	1.97	0.45
1:K:191:ASP:O	2:M:938:LYS:NZ	2.49	0.45
2:M:501:THR:HA	2:M:502:PRO:HD3	1.77	0.45
2:M:758:ARG:HH21	2:M:788:THR:HB	1.81	0.45
3:N:827:ILE:HG22	3:N:829:VAL:HG23	1.97	0.45
3:N:1211:MET:SD	4:O:16:LYS:HE2	2.56	0.45
1:A:8:ALA:HA	1:A:9:PRO:HD3	1.58	0.45
1:A:34:VAL:HG22	1:B:42:ARG:NH2	2.30	0.45
2:C:144:PRO:HB2	2:C:273:GLY:HA3	1.99	0.45
2:C:930:LYS:HE3	2:C:935:GLY:HA2	1.98	0.45
2:C:937:ASP:OD1	2:C:938:LYS:N	2.49	0.45
3:D:30:GLU:OE1	3:D:40:GLU:HG2	2.16	0.45
3:D:796:ARG:HB2	3:D:824:ASN:ND2	2.31	0.45
4:E:83:ASP:OD1	4:E:83:ASP:N	2.50	0.45
2:M:195:LEU:HD23	2:M:238:LEU:HD13	1.98	0.45
1:A:179:PHE:HB3	1:A:197:LEU:CD2	2.47	0.45
2:C:419:THR:HG22	2:C:420:ARG:H	1.80	0.45
2:C:711:GLU:HG2	2:C:822:VAL:HG22	1.99	0.45
3:D:1274:ILE:HB	3:D:1322:GLY:HA2	1.99	0.45
2:M:577:PRO:HB3	2:M:993:PHE:CG	2.52	0.45
2:M:700:TYR:HD2	2:M:996:LYS:HB2	1.82	0.45
3:N:129:PHE:HD1	3:N:456:MET:HE3	1.82	0.45
5:P:84:TYR:O	5:P:88:ILE:HG12	2.16	0.45
1:B:177:VAL:HG13	1:B:197:LEU:HD11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:781:PRO:HG2	3:D:911:LEU:HB3	1.99	0.45
3:N:1429:LEU:HG	3:N:1440:PHE:CD1	2.49	0.45
5:P:354:LEU:O	5:P:358:LEU:HB2	2.15	0.45
5:P:412:GLU:O	5:P:413:SER:O	2.35	0.45
2:C:605:LYS:HD3	2:C:610:ARG:NE	2.31	0.45
2:C:877:PRO:HG3	3:D:1023:MET:CE	2.39	0.45
3:D:71:LYS:O	3:D:80:VAL:HG22	2.17	0.45
3:N:477:LEU:O	3:N:481:MET:HG2	2.16	0.45
5:P:153:PRO:O	5:P:156:VAL:HG22	2.16	0.45
2:C:628:PHE:N	2:C:628:PHE:CD2	2.84	0.45
2:C:704:HIS:CD2	2:C:831:ARG:HG3	2.50	0.45
2:C:853:LEU:HB2	2:C:858:MET:HE2	1.98	0.45
2:M:571:LEU:HD22	2:M:700:TYR:HA	1.98	0.45
3:N:1353:GLN:O	3:N:1357:ARG:HG3	2.16	0.45
5:P:402:ASN:O	5:P:406:ARG:HG3	2.16	0.45
1:B:18:ARG:O	1:B:207:PRO:HD3	2.16	0.45
2:C:939:ARG:H	2:C:939:ARG:HG2	1.47	0.45
3:D:805:GLU:HB3	3:D:828:LYS:HB2	1.99	0.45
3:D:989:TYR:O	3:D:993:LEU:HG	2.17	0.45
3:D:1041:LEU:HD13	3:D:1043:GLY:HA2	1.99	0.45
3:D:1491:THR:HG22	3:D:1495:ILE:HD11	1.98	0.45
3:N:1130:ARG:O	3:N:1131:SER:OG	2.27	0.45
5:P:383:LEU:HD12	5:P:395:GLU:OE1	2.17	0.45
1:A:29:GLU:O	1:A:32:PHE:HB2	2.16	0.45
1:B:71:VAL:HG13	1:B:131:THR:O	2.17	0.45
2:C:374:ASN:HD21	5:F:276:ARG:NH1	2.14	0.45
2:C:569:VAL:HG21	2:C:1000:MET:HE3	1.99	0.45
2:C:971:LYS:NZ	3:D:953:ASP:OD1	2.49	0.45
3:D:126:VAL:O	3:D:457:GLY:N	2.41	0.45
3:D:166:GLN:HB3	3:D:394:LEU:HD11	1.99	0.45
3:D:178:LEU:HG	3:D:192:ALA:HA	1.99	0.45
3:D:367:ILE:HG13	3:D:379:ALA:HB2	1.99	0.45
3:D:371:ILE:HG21	5:F:232:ARG:NH1	2.31	0.45
3:D:1336:LEU:HD13	3:D:1344:VAL:HG21	1.99	0.45
5:F:383:LEU:O	5:F:397:ILE:HG21	2.17	0.45
1:L:201:THR:HG21	1:L:205:VAL:O	2.16	0.45
2:M:719:PRO:HB2	2:M:721:ARG:HD3	1.98	0.45
2:M:757:GLY:HA2	2:M:789:SER:HB3	1.98	0.45
2:M:1056:LYS:O	3:N:624:ASP:N	2.49	0.45
3:N:803:GLY:HA2	3:N:826:PRO:O	2.17	0.45
5:P:233:PHE:CE1	6:R:3:DT:H5"	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:595:LEU:HB2	2:C:656:ALA:HB3	1.99	0.45
2:C:911:GLU:O	2:C:915:LYS:HG2	2.16	0.45
3:D:53:ILE:HG22	3:D:54:LYS:HG3	1.99	0.45
5:F:367:MET:HB3	5:F:390:PHE:CZ	2.48	0.45
2:M:1008:ARG:NH1	2:M:1028:GLY:HA2	2.32	0.45
3:N:101:HIS:HB3	3:N:104:PHE:HD2	1.81	0.45
3:N:520:LEU:HD23	3:N:525:ARG:HG2	1.99	0.45
3:N:849:ALA:O	3:N:853:VAL:HG23	2.16	0.45
5:P:409:LYS:C	5:P:409:LYS:HD3	2.41	0.45
7:Q:18:DA:H2"	7:Q:19:DG:H5"	1.98	0.45
1:A:9:PRO:HB3	1:A:27:PRO:O	2.16	0.45
2:C:550:LEU:HD23	2:C:905:ILE:CG2	2.46	0.45
2:C:958:THR:HG23	2:C:961:GLU:CD	2.42	0.45
3:D:730:PRO:O	3:D:733:CYS:HB2	2.16	0.45
3:D:832:ARG:HG3	3:D:833:GLU:HG2	1.98	0.45
4:E:14:ASP:OD1	4:E:18:ARG:NH1	2.50	0.45
4:E:14:ASP:OD2	4:E:18:ARG:HD2	2.17	0.45
5:F:361:LEU:HB2	5:F:366:ALA:HB2	1.97	0.45
5:F:370:LYS:O	5:F:376:ILE:HG12	2.17	0.45
2:M:154:ARG:HA	2:M:155:PRO:HD3	1.81	0.45
2:M:462:ASP:OD2	2:M:468:ARG:NH1	2.45	0.45
1:A:185:ARG:CZ	1:A:187:GLY:HA2	2.47	0.44
1:B:48:ILE:HA	1:B:49:PRO:HD3	1.75	0.44
2:C:177:GLU:HB3	2:C:178:PRO:HA	1.98	0.44
2:C:1043:TYR:HE1	3:D:710:ARG:O	2.00	0.44
3:D:129:PHE:HD1	3:D:456:MET:HE3	1.82	0.44
3:D:1271:LYS:HG3	3:D:1272:ALA:O	2.17	0.44
2:M:26:TYR:OH	2:M:119:PRO:O	2.30	0.44
2:M:122:THR:OG1	2:M:124:ASP:OD1	2.35	0.44
4:O:37:ASN:HD22	4:O:89:MET:HE1	1.82	0.44
5:P:368:VAL:CG1	5:P:397:ILE:HD11	2.44	0.44
1:A:87:VAL:HG11	1:A:144:VAL:HG11	1.98	0.44
2:C:258:TYR:CD2	2:C:262:ALA:HB3	2.52	0.44
2:C:433:THR:O	2:C:437:ARG:HD2	2.16	0.44
2:C:679:PHE:HB2	2:C:870:ILE:HG21	1.99	0.44
3:D:480:GLU:HG2	3:D:492:ALA:HB2	1.99	0.44
3:D:925:GLU:HG3	4:E:2:ALA:HB3	1.99	0.44
3:D:1486:VAL:HG21	4:E:22:VAL:HG13	1.99	0.44
2:M:80:GLN:HG2	2:M:90:TYR:CE1	2.52	0.44
2:M:874:LEU:HD21	3:N:787:LEU:HD22	2.00	0.44
3:N:213:VAL:HG21	3:N:367:ILE:HD13	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:285:PRO:O	3:N:288:MET:HB3	2.16	0.44
1:B:179:PHE:HB3	1:B:197:LEU:HD13	1.98	0.44
2:C:976:ASP:OD1	2:C:977:GLY:N	2.50	0.44
3:D:1095:THR:O	3:D:1099:VAL:HG23	2.17	0.44
3:D:1235:GLN:O	3:D:1359:GLN:HG2	2.17	0.44
2:M:805:ARG:NH2	2:M:821:GLU:OE1	2.47	0.44
3:N:208:PRO:HA	3:N:390:PRO:HA	1.98	0.44
3:N:1042:ARG:HB3	3:N:1057:VAL:HB	1.99	0.44
1:A:150:TYR:CE1	2:C:696:LYS:HA	2.52	0.44
2:C:239:PHE:CZ	2:C:243:ARG:HD2	2.53	0.44
5:F:163:LEU:HB3	5:F:174:LEU:HD22	1.98	0.44
1:K:24:VAL:HG22	1:K:196:THR:HG23	1.99	0.44
2:M:202:TYR:CE1	2:M:304:LEU:HD22	2.52	0.44
2:M:450:GLY:HA2	3:N:1078:ARG:NH1	2.32	0.44
3:N:238:PRO:HD3	3:N:318:ARG:HG3	1.98	0.44
3:N:388:HIS:O	3:N:390:PRO:HD3	2.17	0.44
1:A:43:ILE:HG12	1:B:32:PHE:CZ	2.52	0.44
2:C:34:VAL:HA	2:C:35:PRO:HD2	1.83	0.44
2:C:679:PHE:HA	3:D:943:THR:HB	1.99	0.44
3:D:463:GLN:OE1	3:D:463:GLN:HA	2.17	0.44
3:D:566:ILE:HD11	5:F:192:LEU:HD21	1.99	0.44
3:D:764:LEU:HD23	3:D:766:ALA:HB3	2.00	0.44
5:F:374:GLY:HA2	5:F:379:ARG:O	2.17	0.44
2:M:657:ASP:OD2	2:M:663:ASN:N	2.47	0.44
3:N:348:GLN:HB3	3:N:349:PRO:HD2	1.99	0.44
1:A:213:GLN:O	1:A:217:ILE:HG13	2.18	0.44
2:C:1072:LYS:HD3	2:C:1074:GLU:OE2	2.17	0.44
3:D:952:ASP:HA	3:D:1062:ARG:NH2	2.33	0.44
5:F:237:THR:HA	6:H:5:DA:N7	2.32	0.44
5:F:333:ILE:HA	5:F:334:PRO:HD3	1.81	0.44
2:M:135:VAL:HG23	2:M:395:LYS:HG3	1.99	0.44
3:N:646:LYS:HB3	3:N:688:TRP:CZ3	2.53	0.44
3:N:696:HIS:HD2	3:N:697:GLY:N	2.15	0.44
2:C:511:GLU:HG3	2:C:512:ARG:HG2	1.98	0.44
2:C:674:VAL:HG21	2:C:871:LEU:HG	1.99	0.44
3:D:18:ILE:CG2	3:D:518:PRO:HG3	2.48	0.44
3:D:209:ARG:NH2	3:D:391:ALA:HA	2.33	0.44
3:D:643:GLY:HA3	3:D:727:GLN:HB2	2.00	0.44
2:M:679:PHE:CE2	2:M:853:LEU:HD11	2.53	0.44
3:N:1127:GLU:CG	3:N:1133:ARG:HB3	2.46	0.44
1:A:20:TYR:C	1:A:207:PRO:HG2	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:38:LYS:HB3	2:C:38:LYS:HE2	1.71	0.44
3:D:271:VAL:HG22	3:D:281:THR:HG23	2.00	0.44
3:D:567:ILE:HA	3:D:567:ILE:HD13	1.58	0.44
3:D:784:ASP:HB2	3:D:939:PHE:HE2	1.83	0.44
3:D:1018:ASN:O	3:D:1022:VAL:HG23	2.17	0.44
3:D:1018:ASN:HA	3:D:1019:PRO:HD3	1.79	0.44
3:D:1376:MET:HE2	3:D:1376:MET:HB3	1.66	0.44
5:F:188:ILE:HD13	5:F:221:ILE:HG12	2.00	0.44
1:K:193:ASP:HB3	2:M:938:LYS:HD2	1.99	0.44
2:M:74:GLY:HA3	2:M:93:PRO:HG2	2.00	0.44
2:M:605:LYS:HB2	2:M:612:VAL:HB	1.99	0.44
2:M:976:ASP:OD2	2:M:978:ARG:NH1	2.50	0.44
2:M:1097:LEU:HD13	3:N:10:ILE:HD11	2.00	0.44
3:N:32:ILE:O	5:P:258:ILE:HG23	2.17	0.44
2:C:212:GLY:HA2	2:C:218:VAL:HG21	2.00	0.44
3:D:14:SER:HB3	3:D:511:TRP:CZ2	2.53	0.44
3:D:242:LEU:HD12	3:D:242:LEU:HA	1.78	0.44
3:D:666:ILE:HG22	3:D:676:MET:HE1	1.99	0.44
3:D:772:PRO:O	3:D:1209:LEU:HD12	2.17	0.44
3:D:1128:VAL:CG2	3:D:1133:ARG:HD3	2.43	0.44
1:L:48:ILE:HG22	1:L:173:PRO:HD2	2.00	0.44
2:M:34:VAL:HA	2:M:35:PRO:HD2	1.83	0.44
2:M:173:ASP:O	2:M:184:MET:HA	2.17	0.44
2:M:759:THR:HB	2:M:785:VAL:HB	1.99	0.44
2:M:976:ASP:OD1	2:M:978:ARG:HD3	2.18	0.44
3:N:821:VAL:HG11	3:N:827:ILE:HD11	2.00	0.44
5:P:222:ARG:HA	5:P:222:ARG:HE	1.82	0.44
1:A:80:LEU:HD23	2:C:573:ARG:HD2	2.00	0.43
1:B:38:ASN:O	1:B:41:ARG:N	2.50	0.43
1:B:57:TYR:CZ	1:B:161:ARG:HD2	2.53	0.43
2:C:99:GLN:O	2:C:99:GLN:HG3	2.18	0.43
2:C:157:ARG:HA	2:C:157:ARG:HD3	1.68	0.43
2:C:363:SER:HB3	2:C:366:SER:H	1.82	0.43
3:D:1352:ILE:HD12	3:D:1368:ILE:HG23	2.00	0.43
5:F:371:LEU:O	5:F:381:HIS:HD2	2.01	0.43
2:M:965:GLU:O	2:M:969:GLN:HG3	2.18	0.43
3:N:209:ARG:N	3:N:389:GLU:O	2.28	0.43
3:N:1144:LEU:O	3:N:1147:ARG:HG3	2.18	0.43
4:O:14:ASP:OD2	4:O:14:ASP:N	2.43	0.43
5:P:373:LYS:HD3	5:P:373:LYS:HA	1.88	0.43
2:C:35:PRO:HA	2:C:36:PRO:HD3	1.88	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:265:GLU:HB3	3:D:266:GLU:H	1.51	0.43
5:F:157:GLU:O	5:F:161:GLN:HG2	2.18	0.43
5:F:285:GLU:HA	5:F:286:PRO:HD3	1.77	0.43
2:M:258:TYR:CD2	2:M:262:ALA:HB3	2.52	0.43
2:M:719:PRO:HB3	2:M:820:ARG:NH2	2.34	0.43
3:N:584:ASN:CG	3:N:590:PRO:HD2	2.43	0.43
3:N:715:ALA:HB3	3:N:764:LEU:HA	2.00	0.43
3:N:1147:ARG:HD3	3:N:1188:VAL:HG11	1.99	0.43
4:O:49:GLN:NE2	4:O:50:THR:O	2.51	0.43
5:P:329:TYR:CE2	5:P:333:ILE:HD11	2.52	0.43
5:P:372:ARG:O	5:P:380:GLU:HB2	2.18	0.43
3:D:128:TYR:OH	3:D:587:ARG:HD2	2.17	0.43
3:D:815:ALA:HA	3:D:818:ARG:CZ	2.48	0.43
3:D:963:TYR:HE2	3:D:1002:LYS:HD3	1.83	0.43
3:D:1144:LEU:HA	3:D:1144:LEU:HD23	1.59	0.43
1:L:115:LEU:O	1:L:117:VAL:HG23	2.19	0.43
2:M:258:TYR:CE2	2:M:293:PHE:HB2	2.53	0.43
2:M:1019:GLN:HG2	2:M:1058:ASP:HB3	2.00	0.43
2:M:1021:LEU:HD22	5:P:331:ASP:O	2.19	0.43
3:N:68:PHE:HB2	3:N:80:VAL:HG21	2.01	0.43
3:N:589:ALA:HB1	3:N:599:PRO:HB3	2.00	0.43
2:C:435:TYR:OH	2:C:533:ASP:OD2	2.33	0.43
2:C:835:VAL:HG13	2:C:849:VAL:O	2.18	0.43
3:D:179:VAL:HG21	3:D:191:LEU:HD12	2.00	0.43
3:D:561:GLY:HA3	5:F:132:ARG:HD3	2.00	0.43
3:D:728:LEU:HD12	3:D:729:HIS:H	1.84	0.43
3:D:998:GLU:O	3:D:1002:LYS:HG3	2.18	0.43
3:D:1256:LEU:O	3:D:1260:ILE:HG13	2.18	0.43
5:F:80:PRO:HB2	5:F:210:LEU:HD11	2.00	0.43
5:F:152:ASP:HB2	5:F:153:PRO:HD2	2.01	0.43
5:P:372:ARG:HD2	5:P:381:HIS:O	2.19	0.43
2:C:144:PRO:HD2	2:C:332:ARG:HD3	2.00	0.43
2:C:767:PRO:HB2	2:C:771:GLU:HB3	2.00	0.43
3:D:1351:GLU:O	3:D:1354:LYS:HB2	2.19	0.43
1:L:75:VAL:O	1:L:79:ILE:HG23	2.17	0.43
7:G:14:DG:H2'	7:G:15:BRU:H6	2.00	0.43
2:C:283:ILE:HG21	2:C:305:PRO:HG2	2.00	0.43
2:C:888:THR:O	2:C:892:LEU:N	2.51	0.43
3:D:787:LEU:HD21	3:D:947:ILE:HG13	2.01	0.43
3:D:1266:ARG:CZ	6:H:18:DC:H5''	2.49	0.43
1:L:138:LEU:HD21	1:L:140:MET:HE3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:905:ILE:HG22	2:M:906:PHE:CD2	2.53	0.43
3:N:158:TYR:CE1	3:N:454:ALA:HB3	2.53	0.43
3:N:411:THR:HA	3:N:435:VAL:HG12	1.99	0.43
3:N:881:LEU:O	3:N:885:ILE:HG13	2.17	0.43
5:P:361:LEU:HD12	5:P:362:SER:H	1.84	0.43
1:A:6:LEU:HD13	1:A:7:LYS:H	1.82	0.43
1:B:149:GLY:HA2	1:B:172:SER:HB2	2.01	0.43
2:C:353:ARG:NH2	6:H:9:DG:H3'	2.29	0.43
2:C:422:ARG:HB3	6:H:15:DT:OP2	2.19	0.43
3:D:140:ALA:CB	3:D:452:ILE:HD12	2.48	0.43
1:K:185:ARG:NH1	1:K:187:GLY:HA2	2.33	0.43
1:L:65:PHE:HZ	3:N:810:GLU:HB2	1.82	0.43
2:M:952:LEU:HB3	2:M:966:LEU:HD21	2.01	0.43
3:N:818:ARG:HB2	3:N:820:GLU:HG3	2.01	0.43
3:N:1377:LYS:HE3	3:N:1378:TYR:CZ	2.53	0.43
5:P:201:LYS:NZ	5:P:244:ARG:HH21	2.17	0.43
2:C:281:LEU:HD22	2:C:305:PRO:O	2.19	0.43
2:C:628:PHE:N	2:C:628:PHE:HD2	2.17	0.43
2:C:899:GLN:HE21	2:C:901:TYR:HE2	1.66	0.43
2:C:958:THR:HG23	2:C:961:GLU:OE1	2.18	0.43
3:D:23:TYR:CD2	3:D:89:ARG:HD3	2.54	0.43
3:D:87:ARG:HG2	3:D:523:ASP:CB	2.49	0.43
3:D:98:PRO:O	3:D:458:ALA:HB3	2.18	0.43
3:D:996:TRP:CD2	3:D:1056:PRO:HG3	2.54	0.43
5:F:166:LEU:HD13	5:F:170:HIS:HB3	2.01	0.43
1:L:40:LEU:HD13	1:L:211:LEU:HD11	2.00	0.43
1:A:6:LEU:HD22	1:A:6:LEU:HA	1.86	0.43
2:C:979:THR:HB	2:C:981:GLU:HG3	2.01	0.43
3:D:272:LEU:O	3:D:279:VAL:N	2.44	0.43
3:D:1348:LEU:O	3:D:1352:ILE:HG13	2.18	0.43
3:D:1432:LYS:O	3:D:1455:LYS:NZ	2.52	0.43
1:L:64:GLU:HG2	1:L:75:VAL:HG11	2.01	0.43
2:M:164:PRO:HB3	2:M:267:TYR:CZ	2.54	0.43
3:N:843:PHE:HE1	3:N:864:VAL:HG11	1.82	0.43
1:A:134:GLU:C	1:A:136:GLY:H	2.26	0.43
1:A:150:TYR:HD1	1:A:170:VAL:HG22	1.84	0.43
1:B:123:MET:C	1:B:125:PRO:HD3	2.44	0.43
2:C:164:PRO:HB2	2:C:168:ARG:O	2.19	0.43
2:C:569:VAL:HG11	2:C:704:HIS:HE1	1.84	0.43
3:D:116:LEU:HD11	3:D:461:ILE:HG23	2.01	0.43
3:D:566:ILE:HD13	5:F:217:ASN:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:984:THR:HG22	3:D:986:ARG:H	1.82	0.43
3:D:1491:THR:O	3:D:1495:ILE:HG13	2.19	0.43
1:K:39:PRO:O	1:K:43:ILE:HG13	2.19	0.43
1:K:53:VAL:HG22	1:K:144:VAL:HG22	2.01	0.43
2:M:818:GLY:HA3	5:P:309:LYS:HD2	2.00	0.43
2:M:1095:LEU:HD13	3:N:103:TRP:CH2	2.54	0.43
3:N:107:ASP:CG	3:N:1445:HIS:HD1	2.26	0.43
3:N:544:TYR:O	3:N:548:ILE:HG12	2.19	0.43
3:N:806:PHE:O	3:N:829:VAL:HA	2.19	0.43
5:P:413:SER:HB3	5:P:414:ARG:H	1.56	0.43
7:G:17:DG:O5'	7:G:17:DG:H8	2.01	0.43
1:A:57:TYR:HE1	1:A:163:ASN:HB2	1.84	0.42
2:C:1001:VAL:HG11	3:D:725:SER:HB3	2.01	0.42
3:D:1281:VAL:O	3:D:1316:GLY:N	2.36	0.42
5:F:338:LEU:HA	5:F:339:PRO:HD3	1.85	0.42
3:N:521:PRO:HA	3:N:522:PRO:HD3	1.79	0.42
3:N:1216:SER:HB3	4:O:16:LYS:H	1.84	0.42
4:O:80:VAL:HG22	4:O:81:PRO:O	2.18	0.42
1:A:57:TYR:CE1	1:A:163:ASN:HB2	2.53	0.42
2:C:3:ILE:CD1	2:C:900:ARG:HG3	2.50	0.42
2:C:139:GLN:HG2	2:C:140:ILE:N	2.34	0.42
2:C:142:ARG:NH2	2:C:325:ILE:HD13	2.33	0.42
2:C:501:THR:HG21	2:C:513:VAL:HB	2.01	0.42
2:C:617:ASP:OD2	2:C:619:ARG:NE	2.53	0.42
3:D:183:GLU:O	3:D:185:VAL:HG23	2.20	0.42
3:D:827:ILE:HG22	3:D:829:VAL:HG23	2.00	0.42
3:D:1263:PHE:HA	3:D:1375:MET:HE1	2.01	0.42
1:K:14:ARG:HB2	1:K:22:GLU:HB2	2.01	0.42
1:K:206:THR:HG23	1:K:207:PRO:HD2	2.01	0.42
1:L:22:GLU:HG2	1:L:198:ARG:HG2	2.01	0.42
2:M:290:LEU:HD23	2:M:302:VAL:HG21	1.99	0.42
4:O:95:VAL:O	4:O:95:VAL:CG1	2.66	0.42
5:P:368:VAL:HG12	5:P:390:PHE:CE1	2.54	0.42
1:B:91:ASN:HA	1:B:92:PRO:HD2	1.79	0.42
2:C:906:PHE:HZ	3:D:1070:TYR:CD2	2.38	0.42
3:D:623:VAL:HG21	3:D:748:HIS:ND1	2.34	0.42
3:D:1130:ARG:CD	3:D:1131:SER:H	2.32	0.42
1:L:79:ILE:HA	1:L:82:LEU:HD12	2.01	0.42
3:N:1413:THR:HG22	3:N:1414:PRO:HD2	2.01	0.42
4:O:42:PRO:HA	4:O:45:ARG:HD2	2.01	0.42
5:P:357:ALA:HA	5:P:360:LYS:HG2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:372:ARG:HA	5:P:381:HIS:O	2.18	0.42
6:H:15:DT:C2'	6:H:16:DC:H5'	2.46	0.42
6:R:14:DG:H2''	6:R:15:DT:H5'	2.01	0.42
1:A:25:LEU:HD21	1:B:224:TYR:CB	2.48	0.42
1:A:88:ARG:HB2	1:A:123:MET:SD	2.59	0.42
2:C:111:ASP:OD1	2:C:370:ALA:HB2	2.19	0.42
2:C:495:THR:HG23	2:C:517:ARG:HG3	2.02	0.42
2:C:557:ARG:NH1	2:C:879:ARG:HG3	2.34	0.42
2:C:719:PRO:O	2:C:761:PHE:HD1	2.02	0.42
3:D:30:GLU:HG2	5:F:259:ARG:CD	2.49	0.42
3:N:264:LEU:O	3:N:264:LEU:HD12	2.19	0.42
3:N:273:ARG:HB2	3:N:275:GLU:O	2.19	0.42
5:P:408:LEU:CD2	5:P:412:GLU:HG2	2.40	0.42
5:P:415:THR:CG2	5:P:416:ARG:CG	2.88	0.42
2:C:605:LYS:HB2	2:C:612:VAL:HB	2.02	0.42
2:C:1092:LEU:HD23	2:C:1092:LEU:HA	1.84	0.42
3:D:90:MET:HB3	3:D:90:MET:HE2	1.61	0.42
3:D:554:LEU:CD2	3:D:574:LEU:HD22	2.49	0.42
3:D:1341:PRO:HG3	3:D:1419:PRO:CB	2.50	0.42
5:F:372:ARG:HE	5:F:383:LEU:HG	1.85	0.42
3:N:245:LEU:HD22	3:N:249:TYR:HB3	2.01	0.42
3:N:1083:ASP:OD1	3:N:1087:ARG:HG3	2.19	0.42
4:O:8:LYS:HE3	4:O:8:LYS:HB2	1.79	0.42
5:P:193:ARG:HB2	6:R:6:DT:H1'	2.01	0.42
2:C:368:THR:HB	2:C:370:ALA:H	1.84	0.42
2:C:710:ILE:HD12	2:C:790:LEU:HB2	2.02	0.42
2:C:881:ASN:OD1	2:C:881:ASN:N	2.46	0.42
2:C:910:LYS:O	2:C:914:ILE:HG13	2.20	0.42
2:C:1039:ALA:HB3	3:D:713:ILE:HD12	2.02	0.42
3:D:925:GLU:O	3:D:928:ALA:HB3	2.20	0.42
5:F:128:ARG:NH2	5:F:129:GLU:OE1	2.53	0.42
1:K:83:LYS:CE	1:K:168:ASP:HB2	2.47	0.42
3:N:517:VAL:HA	3:N:518:PRO:HD3	1.89	0.42
3:N:1236:LEU:CD1	3:N:1355:VAL:HG11	2.50	0.42
6:R:13:DT:H2''	6:R:14:DG:OP2	2.19	0.42
1:A:114:PHE:HE1	1:A:129:ILE:HD11	1.85	0.42
1:A:155:LYS:HD3	1:A:155:LYS:HA	1.82	0.42
1:B:97:VAL:HG12	1:B:98:THR:N	2.34	0.42
2:C:226:VAL:HG13	2:C:227:PHE:CD1	2.55	0.42
2:C:269:LEU:HB2	2:C:288:ARG:O	2.19	0.42
2:C:326:ASP:HA	2:C:331:ARG:HD2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:805:ARG:NH2	2:C:821:GLU:OE1	2.53	0.42
3:D:236:TYR:HB2	3:D:319:ALA:HB3	2.01	0.42
3:D:584:ASN:OD1	3:D:585:GLY:N	2.53	0.42
3:D:826:PRO:C	3:D:827:ILE:HG13	2.45	0.42
2:M:332:ARG:HB3	2:M:466:PHE:CE2	2.55	0.42
3:N:71:LYS:O	3:N:80:VAL:HG22	2.19	0.42
3:N:462:GLN:HB2	3:N:513:ILE:HG21	2.01	0.42
3:N:1280:VAL:HA	3:N:1317:ASP:O	2.20	0.42
5:P:193:ARG:HB3	6:R:7:DG:H5'	2.01	0.42
5:P:357:ALA:HB1	5:P:408:LEU:HD21	2.02	0.42
7:G:16:DC:H5''	7:G:16:DC:H6	1.84	0.42
1:A:86:VAL:HG22	1:A:123:MET:HG3	2.01	0.42
2:C:28:ARG:HH11	2:C:42:VAL:HG21	1.84	0.42
2:C:942:GLU:O	2:C:945:ARG:HB3	2.19	0.42
3:D:227:LEU:HD13	3:D:331:VAL:HG21	2.01	0.42
3:D:241:ILE:HA	3:D:312:ARG:CB	2.50	0.42
3:D:754:PHE:HA	4:E:24:ALA:HB1	2.00	0.42
3:D:1146:GLY:HA3	3:D:1207:TYR:HB2	2.01	0.42
3:D:1275:SER:O	3:D:1322:GLY:N	2.35	0.42
2:M:768:THR:O	2:M:771:GLU:N	2.53	0.42
3:N:315:ARG:H	3:N:315:ARG:HD3	1.85	0.42
3:N:1001:GLU:O	3:N:1005:GLN:HG2	2.20	0.42
3:N:1124:GLN:HA	3:N:1125:PRO:HD3	1.80	0.42
5:P:93:LEU:HD21	5:P:193:ARG:HD3	2.02	0.42
5:P:324:GLU:OE2	5:P:324:GLU:N	2.50	0.42
1:B:8:ALA:HA	1:B:9:PRO:HD3	1.71	0.42
1:B:172:SER:HA	1:B:173:PRO:HD2	1.88	0.42
2:C:22:GLN:OE1	2:C:336:VAL:HG11	2.20	0.42
2:C:295:ASP:HA	2:C:296:GLY:HA2	1.49	0.42
2:C:390:GLN:OE1	2:C:414:GLY:HA2	2.19	0.42
3:D:11:ALA:HA	3:D:1451:ALA:O	2.20	0.42
3:D:237:LYS:HE2	3:D:237:LYS:HB3	1.80	0.42
3:D:475:LYS:O	3:D:478:LEU:HB2	2.20	0.42
3:D:521:PRO:HA	3:D:522:PRO:HD3	1.79	0.42
3:D:930:LEU:O	3:D:933:ALA:HB3	2.20	0.42
3:D:989:TYR:CZ	3:D:993:LEU:HD11	2.55	0.42
1:L:57:TYR:CE1	1:L:163:ASN:HB2	2.52	0.42
2:M:582:GLY:N	2:M:584:GLU:OE2	2.46	0.42
2:M:600:ASP:O	2:M:616:GLU:HG2	2.20	0.42
1:B:44:LEU:O	1:B:174:VAL:HG21	2.19	0.42
2:C:1097:LEU:HD11	3:D:103:TRP:HZ3	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:313:MET:HA	3:D:314:PRO:HD3	1.74	0.42
3:D:907:GLU:HB3	3:D:1026:SER:HA	2.02	0.42
3:D:1053:PHE:CZ	3:D:1072:ILE:HD12	2.55	0.42
3:D:1151:ARG:C	3:D:1162:GLU:HG2	2.45	0.42
4:E:14:ASP:OD2	4:E:14:ASP:N	2.50	0.42
4:E:80:VAL:HG22	4:E:81:PRO:O	2.20	0.42
2:M:304:LEU:HB3	2:M:305:PRO:HD3	2.00	0.42
2:M:380:ALA:O	2:M:384:GLU:HB2	2.19	0.42
3:N:356:PRO:HG2	3:N:359:ALA:HB2	2.01	0.42
3:N:1345:GLU:HG3	3:N:1376:MET:HE2	2.02	0.42
2:C:243:ARG:HA	2:C:244:PRO:HD3	1.81	0.41
2:C:672:VAL:HB	2:C:868:ASP:HB2	2.02	0.41
2:C:1093:GLN:HB3	3:D:21:TRP:CZ3	2.55	0.41
3:D:1438:ALA:O	3:D:1443:THR:HG23	2.20	0.41
5:F:291:ILE:HG22	5:F:295:MET:HG3	2.02	0.41
1:K:29:GLU:O	1:K:32:PHE:HB2	2.20	0.41
2:M:260:LEU:HD12	2:M:260:LEU:HA	1.94	0.41
6:H:21:DA:N6	7:G:7:DT:H3	2.12	0.41
2:C:15:LEU:HA	2:C:16:PRO:HD3	1.91	0.41
2:C:44:ILE:HA	2:C:44:ILE:HD13	1.71	0.41
3:D:3:LYS:HA	3:D:3:LYS:HD2	1.56	0.41
3:D:3:LYS:HE3	3:D:4:GLU:H	1.85	0.41
3:D:95:LEU:HD22	3:D:574:LEU:HD21	2.02	0.41
3:D:103:TRP:HB3	3:D:1448:THR:HG21	2.00	0.41
3:D:659:LYS:HE3	3:D:663:GLU:OE2	2.19	0.41
3:D:1150:ALA:HB3	3:D:1187:PRO:HB2	2.01	0.41
5:F:271:LEU:HD11	5:F:304:VAL:HG13	2.01	0.41
1:L:206:THR:HB	1:L:209:GLU:CD	2.45	0.41
2:M:20:GLU:HG3	2:M:21:ILE:N	2.35	0.41
2:M:272:ALA:HA	2:M:464:LEU:HD12	2.02	0.41
2:M:680:ASP:OD1	3:N:943:THR:HG21	2.20	0.41
3:N:949:ILE:HD11	3:N:1023:MET:HE1	2.03	0.41
3:N:1018:ASN:HA	3:N:1019:PRO:HD3	1.87	0.41
3:N:1168:MET:HE3	3:N:1171:VAL:HB	2.02	0.41
3:N:1190:SER:OG	3:N:1369:GLU:OE1	2.33	0.41
1:A:168:ASP:OD2	2:C:832:LYS:NZ	2.34	0.41
2:C:439:CYS:HA	2:C:440:PRO:HD3	1.69	0.41
3:D:411:THR:HA	3:D:435:VAL:HG12	2.02	0.41
3:D:1045:MET:HE3	3:D:1046:GLN:H	1.85	0.41
2:M:324:ASP:O	2:M:325:ILE:HB	2.20	0.41
2:M:442:GLU:OE1	2:M:541:SER:OG	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:65:ARG:HG3	5:P:378:GLY:O	2.21	0.41
3:N:1236:LEU:CD1	3:N:1355:VAL:HG12	2.51	0.41
5:P:329:TYR:C	5:P:329:TYR:CD2	2.98	0.41
7:Q:14:DG:C2'	7:Q:15:BRU:C5'	2.92	0.41
1:A:227:ASN:OD1	1:A:227:ASN:N	2.54	0.41
2:C:150:PRO:HD3	2:C:322:VAL:HG11	2.02	0.41
2:C:899:GLN:NE2	2:C:901:TYR:HE2	2.19	0.41
3:D:388:HIS:O	3:D:390:PRO:HD3	2.20	0.41
3:D:739:ASP:O	3:D:743:ASP:HB2	2.20	0.41
3:D:1068:LEU:O	3:D:1072:ILE:HG12	2.20	0.41
5:F:309:LYS:HA	5:F:312:GLN:HE21	1.86	0.41
2:M:143:SER:O	2:M:147:TYR:OH	2.22	0.41
2:M:302:VAL:O	2:M:306:THR:HG23	2.20	0.41
3:N:47:GLU:HA	3:N:51:GLY:O	2.20	0.41
3:N:729:HIS:HA	3:N:730:PRO:HD3	1.90	0.41
4:O:57:ASP:HA	4:O:58:PRO:HD3	1.86	0.41
5:P:152:ASP:HB2	5:P:153:PRO:HD2	2.01	0.41
5:P:415:THR:HG22	5:P:416:ARG:H	1.84	0.41
1:B:167:VAL:HG12	1:B:168:ASP:O	2.21	0.41
2:C:756:VAL:HG21	2:C:823:VAL:HG11	2.02	0.41
3:D:111:LYS:HD3	3:D:111:LYS:HA	1.84	0.41
3:D:172:PRO:HB2	3:D:175:VAL:CG2	2.50	0.41
3:D:353:VAL:HG11	3:D:387:LEU:HD11	2.03	0.41
3:D:603:LEU:HA	3:D:603:LEU:HD23	1.69	0.41
3:D:1258:ARG:HH21	3:D:1351:GLU:CG	2.32	0.41
3:D:1258:ARG:NH2	3:D:1351:GLU:HG2	2.34	0.41
5:F:193:ARG:HB2	6:H:6:DT:H1'	2.03	0.41
1:K:206:THR:HG22	1:K:208:LEU:N	2.35	0.41
1:L:151:VAL:HG11	1:L:156:HIS:HB3	2.01	0.41
2:M:639:GLN:HA	2:M:657:ASP:O	2.21	0.41
3:N:114:THR:HG21	3:N:498:VAL:HG21	2.02	0.41
3:N:230:TRP:HA	3:N:243:ALA:HA	2.02	0.41
5:P:333:ILE:HA	5:P:334:PRO:HD3	1.89	0.41
2:C:9:ILE:HD11	2:C:500:ASN:HD22	1.86	0.41
2:C:122:THR:OG1	2:C:124:ASP:OD1	2.39	0.41
2:C:411:SER:HG	2:C:413:LEU:HB2	1.85	0.41
3:D:76:CYS:HB2	3:D:78:VAL:HG23	2.01	0.41
3:D:935:LYS:HB3	3:D:935:LYS:HE2	1.84	0.41
3:D:1256:LEU:O	3:D:1256:LEU:HD12	2.20	0.41
3:D:1379:VAL:HG21	3:D:1400:VAL:HG11	2.03	0.41
5:F:120:THR:HG22	5:F:122:LEU:HD13	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:372:ARG:HD3	5:F:401:GLU:OE2	2.20	0.41
1:L:64:GLU:HG2	1:L:75:VAL:CG1	2.50	0.41
2:M:361:MET:SD	5:P:201:LYS:HD2	2.61	0.41
3:N:45:PHE:CD1	3:N:522:PRO:HB3	2.53	0.41
3:N:508:ARG:HA	3:N:509:PRO:HD3	1.93	0.41
3:N:1127:GLU:CB	3:N:1133:ARG:HB3	2.51	0.41
3:N:1492:LEU:HD12	3:N:1493:LYS:HD2	2.03	0.41
5:P:234:LYS:HE2	5:P:234:LYS:HB3	1.91	0.41
1:B:30:ARG:HA	1:B:193:ASP:OD1	2.21	0.41
1:B:205:VAL:HG12	1:B:206:THR:H	1.86	0.41
2:C:361:MET:SD	5:F:201:LYS:HE3	2.61	0.41
3:D:59:ALA:HB3	3:D:76:CYS:HB2	2.03	0.41
3:D:302:GLN:HB2	3:D:303:PRO:HD2	2.03	0.41
3:D:401:TYR:OH	3:D:430:ASP:HB2	2.21	0.41
3:D:610:LYS:HB3	3:D:610:LYS:HE2	1.68	0.41
3:D:956:ILE:HG12	3:D:1039:CYS:O	2.20	0.41
3:D:1352:ILE:HD12	3:D:1368:ILE:CG2	2.50	0.41
2:M:101:ILE:HG12	2:M:108:ILE:HG22	2.02	0.41
2:M:261:ILE:HG23	2:M:290:LEU:HB2	2.02	0.41
3:N:50:PHE:CD2	3:N:522:PRO:HD3	2.54	0.41
3:N:1238:MET:HG3	3:N:1253:THR:CB	2.48	0.41
3:N:1434:TRP:NE1	3:N:1457:ASP:HB2	2.36	0.41
5:P:278:LEU:HD11	5:P:294:ALA:HB3	2.03	0.41
1:A:34:VAL:HG22	1:B:42:ARG:CZ	2.51	0.41
2:C:861:LEU:HD12	2:C:865:THR:OG1	2.20	0.41
3:D:115:LEU:HD23	3:D:115:LEU:HA	1.75	0.41
3:D:631:ILE:CG2	3:D:745:MET:HB2	2.51	0.41
3:D:637:LEU:O	3:D:729:HIS:HD2	2.03	0.41
3:D:1377:LYS:HE3	3:D:1378:TYR:CZ	2.56	0.41
5:F:304:VAL:O	5:F:308:LEU:HG	2.20	0.41
2:M:719:PRO:HB3	2:M:820:ARG:CZ	2.51	0.41
3:N:1133:ARG:HG2	3:N:1134:LEU:N	2.34	0.41
5:P:95:THR:OG1	5:P:97:GLU:OE1	2.28	0.41
5:P:411:HIS:O	5:P:415:THR:OG1	2.38	0.41
2:C:88:LEU:HD23	2:C:813:VAL:HG23	2.03	0.41
2:C:150:PRO:HA	2:C:158:TYR:CD1	2.56	0.41
2:C:184:MET:HE2	2:C:191:PHE:CE2	2.55	0.41
2:C:397:GLU:HB3	2:C:403:SER:CB	2.51	0.41
2:C:411:SER:OG	2:C:413:LEU:HB2	2.21	0.41
2:C:436:GLY:O	2:C:459:ALA:HB2	2.20	0.41
2:C:502:PRO:HB2	2:C:509:ALA:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:550:LEU:HD23	2:C:905:ILE:HG21	2.02	0.41
2:C:712:ALA:O	2:C:820:ARG:HB3	2.20	0.41
2:C:931:GLY:C	2:C:933:GLY:H	2.29	0.41
2:C:1038:TRP:CE2	3:D:1099:VAL:HG11	2.56	0.41
3:D:481:MET:HE3	3:D:481:MET:HB3	1.94	0.41
3:D:869:MET:HE3	3:D:894:LYS:NZ	2.36	0.41
3:D:959:GLU:HB3	3:D:963:TYR:CD1	2.55	0.41
3:D:1143:GLY:O	3:D:1147:ARG:HD2	2.21	0.41
3:D:1447:LEU:HD23	3:D:1447:LEU:HA	1.75	0.41
4:E:57:ASP:HA	4:E:58:PRO:HD3	1.85	0.41
5:F:233:PHE:CD2	6:H:2:DA:H1'	2.56	0.41
1:L:176:ARG:NH2	3:N:888:GLU:OE1	2.54	0.41
2:M:404:LEU:O	2:M:408:ARG:HG3	2.21	0.41
2:M:560:MET:HE2	2:M:846:LYS:NZ	2.36	0.41
2:M:627:ARG:HA	2:M:627:ARG:HD3	1.94	0.41
2:M:878:SER:HB2	3:N:1029:ARG:HD2	2.03	0.41
2:M:936:VAL:HG11	2:M:959:PRO:HB2	2.03	0.41
3:N:226:PRO:HD3	3:N:249:TYR:CE1	2.56	0.41
3:N:269:PHE:CE2	3:N:283:PHE:HD1	2.38	0.41
3:N:631:ILE:HG13	3:N:740:PHE:HD2	1.85	0.41
3:N:832:ARG:C	3:N:833:GLU:HG2	2.46	0.41
3:N:1248:GLY:C	3:N:1250:ALA:H	2.27	0.41
5:P:412:GLU:O	5:P:415:THR:N	2.54	0.41
1:B:20:TYR:CG	1:B:21:GLY:N	2.88	0.41
1:B:173:PRO:O	1:B:201:THR:HG23	2.21	0.41
2:C:160:ALA:O	2:C:173:ASP:HA	2.21	0.41
2:C:644:VAL:HG22	2:C:645:VAL:HG23	2.02	0.41
3:D:591:VAL:HB	3:D:593:ASN:O	2.21	0.41
5:F:223:ALA:HB2	5:F:242:TRP:HB2	2.02	0.41
2:M:905:ILE:C	2:M:907:ASP:H	2.29	0.41
2:M:974:LEU:HD12	2:M:974:LEU:HA	1.95	0.41
3:N:102:ILE:HB	3:N:579:ASP:OD1	2.21	0.41
3:N:480:GLU:HG2	3:N:492:ALA:HB2	2.03	0.41
3:N:658:LEU:HD23	3:N:661:MET:CE	2.51	0.41
3:N:778:LEU:HD23	3:N:778:LEU:HA	1.89	0.41
3:N:984:THR:HB	3:N:987:GLU:H	1.86	0.41
3:N:1232:PRO:O	3:N:1233:GLY:C	2.64	0.41
1:A:20:TYR:CD2	1:A:21:GLY:N	2.89	0.40
1:A:50:GLY:HA3	1:A:173:PRO:HD3	2.04	0.40
1:A:91:ASN:HA	1:A:92:PRO:HD3	1.89	0.40
1:B:101:LEU:HD12	1:B:113:ASP:C	2.46	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:200:LEU:HD22	2:C:300:ASP:HB2	2.02	0.40
2:C:628:PHE:H	2:C:638:ASP:CB	2.34	0.40
2:C:755:LEU:HD22	2:C:825:VAL:HG11	2.03	0.40
3:D:31:THR:OG1	3:D:32:ILE:N	2.54	0.40
3:D:366:LYS:HD3	3:D:369:ALA:HB2	2.03	0.40
3:D:415:VAL:N	3:D:433:GLY:O	2.37	0.40
3:D:1033:GLN:O	3:D:1037:GLN:HG3	2.21	0.40
3:D:1283:ILE:HD12	3:D:1315:ASP:CG	2.46	0.40
3:D:1495:ILE:HG21	4:E:84:ARG:HB3	2.03	0.40
1:K:151:VAL:HA	1:K:152:PRO:HD3	1.86	0.40
1:L:74:ASP:O	1:L:78:ILE:HG13	2.20	0.40
4:O:87:LYS:HA	4:O:87:LYS:HD3	1.88	0.40
2:C:454:SER:HB3	2:C:541:SER:HB2	2.03	0.40
2:C:859:PRO:O	2:C:867:VAL:HG22	2.22	0.40
2:C:1054:THR:C	2:C:1059:ASP:HB3	2.45	0.40
3:D:1364:HIS:ND1	3:D:1366:LYS:HB2	2.36	0.40
5:F:125:ASP:O	5:F:129:GLU:HG2	2.21	0.40
2:M:368:THR:O	2:M:372:LEU:HB2	2.22	0.40
2:M:478:VAL:HG13	2:M:506:ASN:HB3	2.02	0.40
3:N:220:ARG:HH11	3:N:334:THR:HG21	1.86	0.40
3:N:1057:VAL:HG13	3:N:1069:GLU:HB3	2.02	0.40
1:A:115:LEU:HA	1:A:116:PRO:HD3	1.85	0.40
1:B:63:HIS:C	1:B:65:PHE:H	2.28	0.40
3:D:204:LEU:HD23	3:D:441:ARG:NH1	2.36	0.40
3:D:1232:PRO:CB	3:D:1361:VAL:HG11	2.52	0.40
3:D:1282:ARG:HB3	3:D:1293:PHE:HB2	2.03	0.40
3:D:1307:LYS:O	3:D:1307:LYS:HG2	2.22	0.40
4:E:37:ASN:HD22	4:E:89:MET:HE1	1.87	0.40
4:E:49:GLN:NE2	4:E:50:THR:O	2.55	0.40
5:F:95:THR:HG22	5:F:96:LEU:N	2.36	0.40
1:K:10:VAL:HG22	1:K:26:GLU:O	2.21	0.40
1:K:99:LEU:HB3	1:K:114:PHE:CD2	2.56	0.40
2:M:194:VAL:HG22	2:M:221:LEU:HG	2.03	0.40
2:M:1071:ILE:HD13	2:M:1071:ILE:HA	1.96	0.40
3:N:128:TYR:OH	3:N:587:ARG:HD2	2.21	0.40
3:N:322:VAL:HG12	3:N:335:LEU:HD23	2.02	0.40
3:N:845:ASN:HB2	3:N:846:PRO:HD2	2.03	0.40
3:N:996:TRP:CE2	3:N:1056:PRO:HG3	2.56	0.40
3:N:1353:GLN:NE2	3:N:1363:LEU:O	2.48	0.40
3:N:1379:VAL:HG21	3:N:1400:VAL:HG11	2.03	0.40
5:P:172:ARG:O	5:P:176:ILE:HG12	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:R:10:DA:H2''	6:R:11:DG:O4'	2.21	0.40
2:C:606:VAL:HB	2:C:645:VAL:HG22	2.03	0.40
2:C:705:ILE:HG13	2:C:828:ALA:HB2	2.03	0.40
2:C:792:VAL:HA	2:C:793:PRO:HD3	1.92	0.40
3:D:111:LYS:HG3	3:D:1452:ILE:HD11	2.04	0.40
3:D:536:ALA:HA	5:F:315:VAL:O	2.21	0.40
3:D:756:GLN:HB3	4:E:61:VAL:HG21	2.02	0.40
3:D:1197:ARG:HG3	3:D:1398:TRP:CE2	2.56	0.40
5:F:126:LEU:O	5:F:130:VAL:HG23	2.21	0.40
5:F:394:ARG:HG3	5:F:395:GLU:N	2.35	0.40
1:K:32:PHE:HA	1:K:35:THR:HB	2.02	0.40
2:M:729:LEU:HD23	2:M:729:LEU:HA	1.82	0.40
2:M:1050:GLN:O	2:M:1054:THR:OG1	2.26	0.40
3:N:633:VAL:HG13	3:N:635:PRO:HD3	2.03	0.40
3:N:1306:PRO:C	3:N:1308:GLU:H	2.29	0.40
1:B:154:GLU:HG2	3:D:840:LYS:NZ	2.36	0.40
2:C:690:ILE:HD13	2:C:690:ILE:HA	1.84	0.40
2:C:1021:LEU:O	2:C:1028:GLY:HA3	2.21	0.40
3:D:114:THR:HG23	3:D:495:ARG:HG2	2.03	0.40
3:D:631:ILE:HG13	3:D:740:PHE:HD2	1.86	0.40
3:D:712:GLY:C	3:D:736:PHE:HE1	2.29	0.40
3:D:756:GLN:O	3:D:760:ARG:HG3	2.22	0.40
3:D:1139:ASP:OD1	3:D:1357:ARG:HD3	2.22	0.40
2:M:165:LEU:HD23	2:M:165:LEU:HA	1.95	0.40
3:N:716:PHE:HZ	3:N:732:VAL:HG21	1.86	0.40
3:N:963:TYR:HE2	3:N:1002:LYS:HD3	1.86	0.40
3:N:1277:ILE:HG22	3:N:1278:ASP:N	2.36	0.40
3:N:1315:ASP:OD1	3:N:1315:ASP:N	2.54	0.40
3:N:1406:ARG:O	3:N:1410:GLU:HB2	2.22	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 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	224/315 (71%)	219 (98%)	3 (1%)	2 (1%)	14	46
1	B	220/315 (70%)	209 (95%)	11 (5%)	0	100	100
1	K	224/315 (71%)	220 (98%)	4 (2%)	0	100	100
1	L	223/315 (71%)	214 (96%)	9 (4%)	0	100	100
2	C	1107/1119 (99%)	1066 (96%)	40 (4%)	1 (0%)	48	79
2	M	1107/1119 (99%)	1065 (96%)	40 (4%)	2 (0%)	43	73
3	D	1478/1524 (97%)	1418 (96%)	59 (4%)	1 (0%)	48	79
3	N	1485/1524 (97%)	1423 (96%)	59 (4%)	3 (0%)	43	73
4	E	92/99 (93%)	88 (96%)	4 (4%)	0	100	100
4	O	92/99 (93%)	88 (96%)	4 (4%)	0	100	100
5	F	344/443 (78%)	337 (98%)	7 (2%)	0	100	100
5	P	345/443 (78%)	331 (96%)	12 (4%)	2 (1%)	21	55
All	All	6941/7630 (91%)	6678 (96%)	252 (4%)	11 (0%)	43	73

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	325	ILE
2	M	295	ASP
2	M	325	ILE
5	P	413	SER
3	N	1234	THR
5	P	80	PRO
3	N	1087	ARG
3	D	440	VAL
1	A	59	GLU
1	A	226	SER
3	N	440	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	199/273 (73%)	181 (91%)	18 (9%)	9	32
1	B	195/273 (71%)	179 (92%)	16 (8%)	10	34
1	K	199/273 (73%)	187 (94%)	12 (6%)	17	43
1	L	198/273 (72%)	191 (96%)	7 (4%)	32	54
2	C	936/941 (100%)	846 (90%)	90 (10%)	8	29
2	M	936/941 (100%)	900 (96%)	36 (4%)	29	53
3	D	1250/1279 (98%)	1118 (89%)	132 (11%)	6	26
3	N	1253/1279 (98%)	1187 (95%)	66 (5%)	20	45
4	E	83/88 (94%)	74 (89%)	9 (11%)	6	25
4	O	83/88 (94%)	81 (98%)	2 (2%)	43	62
5	F	301/388 (78%)	293 (97%)	8 (3%)	39	59
5	P	302/388 (78%)	281 (93%)	21 (7%)	14	40
All	All	5935/6484 (92%)	5518 (93%)	417 (7%)	14	40

All (417) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	12	THR
1	A	34	VAL
1	A	61	VAL
1	A	76	VAL
1	A	86	VAL
1	A	87	VAL
1	A	122	ILE
1	A	134	GLU
1	A	142	VAL
1	A	158	ILE
1	A	184	THR
1	A	188	GLN
1	A	189	ARG
1	A	198	ARG
1	A	206	THR
1	A	227	ASN
1	A	229	GLN
1	B	15	THR
1	B	34	VAL
1	B	62	LEU
1	B	78	ILE

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Mol	Chain	Res	Type
1	B	82	LEU
1	B	94	LEU
1	B	120	VAL
1	B	158	ILE
1	B	165	ILE
1	B	172	SER
1	B	184	THR
1	B	185	ARG
1	B	192	LEU
1	B	193	ASP
1	B	206	THR
1	B	223	THR
2	C	2	GLU
2	C	10	ARG
2	C	11	GLU
2	C	12	VAL
2	C	13	ILE
2	C	15	LEU
2	C	19	THR
2	C	21	ILE
2	C	27	ARG
2	C	40	GLU
2	C	44	ILE
2	C	113	VAL
2	C	122	THR
2	C	135	VAL
2	C	138	SER
2	C	140	ILE
2	C	149	THR
2	C	159	ILE
2	C	196	LEU
2	C	276	LYS
2	C	281	LEU
2	C	285	LEU
2	C	289	THR
2	C	311	PHE
2	C	336	VAL
2	C	341	THR
2	C	357	GLU
2	C	360	LEU
2	C	366	SER
2	C	368	THR

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Mol	Chain	Res	Type
2	C	403	SER
2	C	418	LEU
2	C	419	THR
2	C	420	ARG
2	C	427	VAL
2	C	429	ASP
2	C	430	VAL
2	C	432	ARG
2	C	433	THR
2	C	445	GLU
2	C	487	THR
2	C	516	ARG
2	C	528	GLU
2	C	530	GLU
2	C	539	VAL
2	C	545	ASN
2	C	557	ARG
2	C	560	MET
2	C	581	THR
2	C	584	GLU
2	C	606	VAL
2	C	607	ASP
2	C	617	ASP
2	C	626	ARG
2	C	628	PHE
2	C	633	GLN
2	C	644	VAL
2	C	645	VAL
2	C	654	LEU
2	C	657	ASP
2	C	674	VAL
2	C	680	ASP
2	C	695	LEU
2	C	710	ILE
2	C	715	THR
2	C	774	LEU
2	C	775	ARG
2	C	788	THR
2	C	789	SER
2	C	801	VAL
2	C	822	VAL
2	C	834	GLN

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Mol	Chain	Res	Type
2	C	845	ASN
2	C	863	ASP
2	C	879	ARG
2	C	900	ARG
2	C	902	ILE
2	C	905	ILE
2	C	929	ARG
2	C	930	LYS
2	C	939	ARG
2	C	950	LEU
2	C	958	THR
2	C	978	ARG
2	C	979	THR
2	C	1001	VAL
2	C	1016	ILE
2	C	1076	VAL
2	C	1099	VAL
2	C	1101	THR
3	D	12	LEU
3	D	30	GLU
3	D	32	ILE
3	D	37	LEU
3	D	47	GLU
3	D	67	ARG
3	D	69	GLU
3	D	81	THR
3	D	83	SER
3	D	90	MET
3	D	93	ILE
3	D	101	HIS
3	D	108	VAL
3	D	121	THR
3	D	141	ILE
3	D	153	LEU
3	D	171	LEU
3	D	179	VAL
3	D	184	GLU
3	D	191	LEU
3	D	199	LEU
3	D	200	ASP
3	D	230	TRP
3	D	231	VAL

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Mol	Chain	Res	Type
3	D	254	GLU
3	D	258	VAL
3	D	265	GLU
3	D	269	PHE
3	D	270	LEU
3	D	273	ARG
3	D	335	LEU
3	D	352	ASN
3	D	354	VAL
3	D	357	GLU
3	D	372	ASP
3	D	387	LEU
3	D	400	VAL
3	D	407	VAL
3	D	411	THR
3	D	415	VAL
3	D	421	LEU
3	D	423	ASP
3	D	428	LYS
3	D	431	VAL
3	D	435	VAL
3	D	441	ARG
3	D	488	ARG
3	D	493	ARG
3	D	513	ILE
3	D	525	ARG
3	D	527	MET
3	D	567	ILE
3	D	578	VAL
3	D	586	ARG
3	D	608	SER
3	D	632	VAL
3	D	633	VAL
3	D	637	LEU
3	D	647	ARG
3	D	666	ILE
3	D	685	ASP
3	D	700	VAL
3	D	720	LEU
3	D	733	CYS
3	D	747	VAL
3	D	756	GLN

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Mol	Chain	Res	Type
3	D	762	GLN
3	D	764	LEU
3	D	778	LEU
3	D	782	SER
3	D	805	GLU
3	D	858	VAL
3	D	864	VAL
3	D	886	VAL
3	D	900	ILE
3	D	907	GLU
3	D	914	LEU
3	D	927	THR
3	D	940	THR
3	D	971	LEU
3	D	980	MET
3	D	983	LEU
3	D	984	THR
3	D	988	ARG
3	D	1012	GLU
3	D	1015	TYR
3	D	1017	PHE
3	D	1029	ARG
3	D	1031	ASN
3	D	1047	LYS
3	D	1055	VAL
3	D	1060	SER
3	D	1067	VAL
3	D	1086	LEU
3	D	1095	THR
3	D	1112	CYS
3	D	1130	ARG
3	D	1131	SER
3	D	1183	ILE
3	D	1188	VAL
3	D	1190	SER
3	D	1200	VAL
3	D	1201	CYS
3	D	1207	TYR
3	D	1211	MET
3	D	1216	SER
3	D	1234	THR
3	D	1237	THR

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Mol	Chain	Res	Type
3	D	1260	ILE
3	D	1274	ILE
3	D	1277	ILE
3	D	1278	ASP
3	D	1282	ARG
3	D	1283	ILE
3	D	1291	SER
3	D	1315	ASP
3	D	1326	THR
3	D	1330	ILE
3	D	1344	VAL
3	D	1366	LYS
3	D	1373	ARG
3	D	1395	LEU
3	D	1403	LEU
3	D	1433	SER
3	D	1439	SER
3	D	1443	THR
3	D	1444	THR
3	D	1460	ILE
3	D	1468	LEU
3	D	1486	VAL
3	D	1488	ASP
3	D	1497	GLU
4	E	15	SER
4	E	19	LEU
4	E	37	ASN
4	E	50	THR
4	E	68	LEU
4	E	74	VAL
4	E	83	ASP
4	E	92	LEU
4	E	95	VAL
5	F	88	ILE
5	F	120	THR
5	F	125	ASP
5	F	138	SER
5	F	295	MET
5	F	338	LEU
5	F	376	ILE
5	F	386	VAL
1	K	6	LEU

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Mol	Chain	Res	Type
1	K	34	VAL
1	K	61	VAL
1	K	76	VAL
1	K	86	VAL
1	K	87	VAL
1	K	134	GLU
1	K	142	VAL
1	K	184	THR
1	K	189	ARG
1	K	206	THR
1	K	215	VAL
1	L	5	LYS
1	L	34	VAL
1	L	158	ILE
1	L	165	ILE
1	L	184	THR
1	L	197	LEU
1	L	206	THR
2	M	11	GLU
2	M	102	HIS
2	M	108	ILE
2	M	113	VAL
2	M	149	THR
2	M	194	VAL
2	M	196	LEU
2	M	218	VAL
2	M	276	LYS
2	M	295	ASP
2	M	297	GLU
2	M	342	ASP
2	M	402	SER
2	M	418	LEU
2	M	427	VAL
2	M	453	THR
2	M	454	SER
2	M	480	THR
2	M	583	LEU
2	M	584	GLU
2	M	607	ASP
2	M	617	ASP
2	M	633	GLN
2	M	670	GLN

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Mol	Chain	Res	Type
2	M	702	SER
2	M	715	THR
2	M	781	LYS
2	M	815	LEU
2	M	905	ILE
2	M	930	LYS
2	M	939	ARG
2	M	968	LEU
2	M	978	ARG
2	M	1001	VAL
2	M	1010	THR
2	M	1080	SER
3	N	35	ARG
3	N	36	THR
3	N	81	THR
3	N	133	ILE
3	N	153	LEU
3	N	184	GLU
3	N	199	LEU
3	N	211	VAL
3	N	245	LEU
3	N	264	LEU
3	N	266	GLU
3	N	270	LEU
3	N	286	VAL
3	N	306	GLU
3	N	311	LEU
3	N	354	VAL
3	N	372	ASP
3	N	400	VAL
3	N	411	THR
3	N	415	VAL
3	N	450	TYR
3	N	480	GLU
3	N	486	ARG
3	N	488	ARG
3	N	525	ARG
3	N	586	ARG
3	N	618	LEU
3	N	637	LEU
3	N	640	HIS
3	N	650	LEU

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Mol	Chain	Res	Type
3	N	709	HIS
3	N	747	VAL
3	N	754	PHE
3	N	780	LYS
3	N	782	SER
3	N	864	VAL
3	N	907	GLU
3	N	940	THR
3	N	949	ILE
3	N	969	ARG
3	N	971	LEU
3	N	1055	VAL
3	N	1067	VAL
3	N	1087	ARG
3	N	1127	GLU
3	N	1130	ARG
3	N	1149	LEU
3	N	1188	VAL
3	N	1194	CYS
3	N	1196	THR
3	N	1200	VAL
3	N	1216	SER
3	N	1236	LEU
3	N	1237	THR
3	N	1238	MET
3	N	1315	ASP
3	N	1326	THR
3	N	1373	ARG
3	N	1382	THR
3	N	1389	LEU
3	N	1390	LEU
3	N	1413	THR
3	N	1433	SER
3	N	1439	SER
3	N	1441	GLN
3	N	1444	THR
4	O	16	LYS
4	O	50	THR
5	P	77	THR
5	P	120	THR
5	P	125	ASP
5	P	156	VAL

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Mol	Chain	Res	Type
5	P	224	VAL
5	P	262	VAL
5	P	271	LEU
5	P	315	VAL
5	P	329	TYR
5	P	340	SER
5	P	358	LEU
5	P	361	LEU
5	P	369	LEU
5	P	377	ASP
5	P	383	LEU
5	P	412	GLU
5	P	413	SER
5	P	414	ARG
5	P	415	THR
5	P	416	ARG
5	P	418	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	212	ASN
1	A	229	GLN
1	B	91	ASN
2	C	99	GLN
2	C	187	ASN
2	C	320	HIS
2	C	374	ASN
2	C	500	ASN
2	C	538	GLN
2	C	543	ASN
2	C	639	GLN
2	C	704	HIS
2	C	899	GLN
3	D	352	ASN
3	D	762	GLN
3	D	824	ASN
3	D	1014	ASN
3	D	1172	HIS
3	D	1489	GLN
4	E	33	HIS
1	K	188	GLN

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Mol	Chain	Res	Type
1	L	212	ASN
2	M	41	ASN
2	M	117	HIS
2	M	187	ASN
2	M	991	GLN
3	N	350	HIS
3	N	483	HIS
3	N	1116	ASN
3	N	1404	ASN
3	N	1442	ASN
5	P	90	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	BRU	Q	15	7	18,21,22	2.77	8 (44%)	25,30,33	2.14	5 (20%)
7	BRU	G	15	7	18,21,22	2.78	8 (44%)	25,30,33	2.17	5 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	BRU	Q	15	7	-	0/7/21/22	0/2/2/2
7	BRU	G	15	7	-	2/7/21/22	0/2/2/2

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	15	BRU	O4-C4	6.81	1.36	1.23
7	Q	15	BRU	O4-C4	6.79	1.36	1.23
7	G	15	BRU	C6-N1	5.38	1.47	1.38
7	Q	15	BRU	C6-N1	5.36	1.47	1.38
7	Q	15	BRU	C2-N1	3.52	1.44	1.38
7	G	15	BRU	C2-N1	3.51	1.44	1.38
7	G	15	BRU	C2-N3	3.35	1.43	1.38
7	Q	15	BRU	C2-N3	3.31	1.43	1.38
7	G	15	BRU	O4'-C4'	-2.83	1.38	1.45
7	Q	15	BRU	O4'-C4'	-2.80	1.38	1.45
7	Q	15	BRU	BR-C5	2.72	1.94	1.88
7	G	15	BRU	BR-C5	2.72	1.94	1.88
7	Q	15	BRU	C4-C5	2.24	1.49	1.45
7	G	15	BRU	C4-C5	2.20	1.49	1.45
7	G	15	BRU	C2'-C3'	-2.14	1.47	1.52
7	Q	15	BRU	C2'-C3'	-2.13	1.47	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	15	BRU	C5-C4-N3	5.83	120.05	113.34
7	Q	15	BRU	C5-C4-N3	5.75	119.95	113.34
7	G	15	BRU	C4-N3-C2	-5.64	119.94	127.34
7	Q	15	BRU	C4-N3-C2	-5.58	120.02	127.34
7	G	15	BRU	O4-C4-C5	-4.59	119.95	125.80
7	Q	15	BRU	O4-C4-C5	-4.53	120.02	125.80
7	G	15	BRU	N3-C2-N1	3.96	120.04	114.89
7	Q	15	BRU	N3-C2-N1	3.92	119.99	114.89
7	G	15	BRU	O2-C2-N1	-2.16	119.99	122.80
7	Q	15	BRU	O2-C2-N1	-2.15	120.00	122.80

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	G	15	BRU	C3'-C4'-C5'-O5'
7	G	15	BRU	O4'-C4'-C5'-O5'

There are no ring outliers.

2 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	Q	15	BRU	10	0
7	G	15	BRU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 6 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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	226/315 (71%)	-0.85	0	100	100	112, 138, 163, 174	0
1	B	222/315 (70%)	-0.78	0	100	100	110, 145, 190, 215	0
1	K	226/315 (71%)	-0.74	0	100	100	114, 145, 171, 193	0
1	L	225/315 (71%)	-0.69	0	100	100	114, 150, 198, 222	0
2	C	1111/1119 (99%)	-0.66	0	100	100	89, 136, 212, 240	0
2	M	1111/1119 (99%)	-0.48	4 (0%)	88	75	98, 154, 239, 269	0
3	D	1482/1524 (97%)	-0.73	1 (0%)	92	87	86, 136, 196, 258	1 (0%)
3	N	1489/1524 (97%)	-0.63	1 (0%)	92	87	84, 139, 199, 263	1 (0%)
4	E	94/99 (94%)	-0.60	0	100	100	107, 138, 175, 185	0
4	O	94/99 (94%)	-0.61	0	100	100	109, 141, 191, 201	0
5	F	346/443 (78%)	-0.53	0	100	100	112, 152, 238, 251	0
5	P	347/443 (78%)	-0.41	3 (0%)	81	61	117, 161, 253, 290	0
6	H	24/27 (88%)	-0.22	0	100	100	144, 191, 241, 247	0
6	R	24/27 (88%)	-0.32	0	100	100	142, 204, 241, 254	0
7	G	15/21 (71%)	-0.32	0	100	100	143, 181, 229, 233	0
7	Q	15/21 (71%)	-0.26	0	100	100	154, 197, 234, 235	0
All	All	7051/7726 (91%)	-0.63	9 (0%)	92	87	84, 144, 219, 290	2 (0%)

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	M	196	LEU	4.8
3	N	353	VAL	3.1
3	D	302	GLN	2.6
2	M	307	LEU	2.2
5	P	357	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
2	M	594	ALA	2.2
5	P	418	LEU	2.2
2	M	306	THR	2.1
5	P	375	LEU	2.1

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	BRU	Q	15	20/21	0.88	0.08	177,196,247,303	1
7	BRU	G	15	20/21	0.94	0.07	138,145,192,257	1

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
9	MG	D	2003	1/1	0.96	0.04	111,111,111,111	0
9	MG	N	2003	1/1	0.98	0.04	127,127,127,127	0
8	ZN	D	2002	1/1	0.99	0.02	164,164,164,164	0
8	ZN	N	2001	1/1	0.99	0.03	166,166,166,166	0
8	ZN	D	2001	1/1	1.00	0.02	168,168,168,168	0
8	ZN	N	2002	1/1	1.00	0.03	138,138,138,138	0

6.5 Other polymers [i](#)

There are no such residues in this entry.