Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 01:41 PM GMT

PDB ID	:	3U5Z
Title	:	Structure of T4 Bacteriophage clamp loader bound to the T4 clamp, primer-template DNA, and ATP analog
Authors	:	Kelch, B.A.; Makino, D.L.; O'Donnell, M.; Kuriyan, J.
Deposited on	:	2011-10-11
Resolution	:	3.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

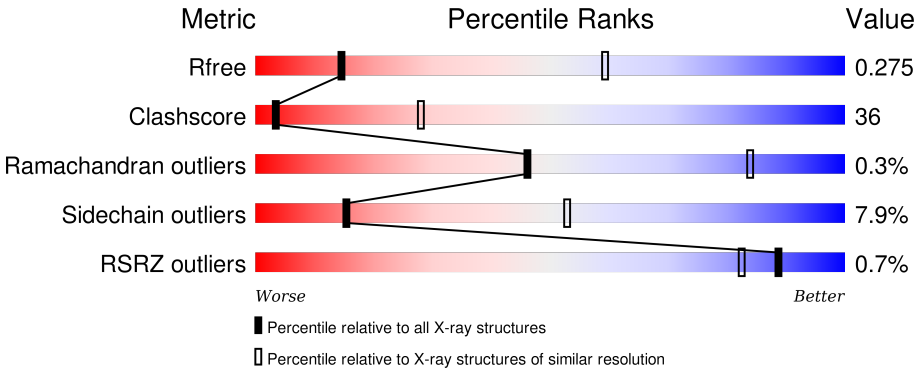
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1051 (3.60-3.40)
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (3.60-3.40)

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

Mol	Chain	Length	Quality of chain
1	B	324	50% 45%
1	C	324	% 51% 44%
1	D	324	47% 49%
1	E	324	% 39% 51% 6%
1	L	324	% 53% 41% 5%

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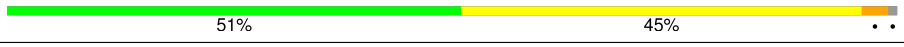
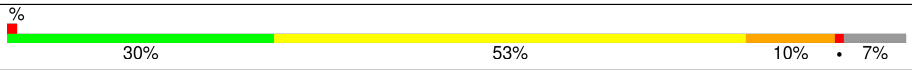
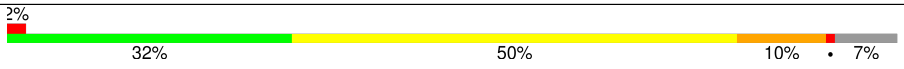
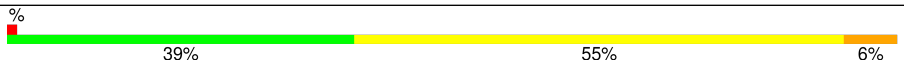
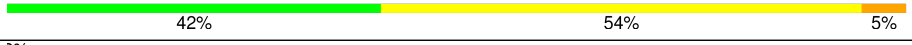
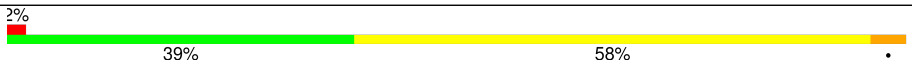
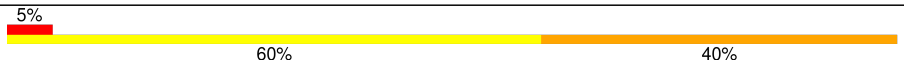
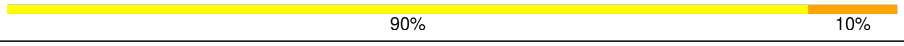
Mol	Chain	Length	Quality of chain
1	M	324	
1	N	324	
1	O	324	
2	A	199	
2	K	199	
3	F	228	
3	G	228	
3	H	228	
3	P	228	
3	Q	228	
3	R	228	
4	I	30	
4	S	30	
5	J	20	
5	T	20	

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
6	08T	M	700	-	-	X	-
7	MG	B	800	-	-	-	X
7	MG	D	800	-	-	-	X
7	MG	L	800	-	-	-	X
7	MG	M	800	-	-	-	X
7	MG	N	800	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 35424 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 polymerase accessory protein 44.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	320	Total	C	N	O	S	0	0	0
			2514	1590	432	475	17			
1	C	320	Total	C	N	O	S	0	0	0
			2514	1590	432	475	17			
1	D	320	Total	C	N	O	S	0	0	0
			2514	1590	432	475	17			
1	E	305	Total	C	N	O	S	0	0	0
			2408	1527	413	452	16			
1	L	320	Total	C	N	O	S	0	0	0
			2514	1590	432	475	17			
1	M	320	Total	C	N	O	S	0	0	0
			2514	1590	432	475	17			
1	N	320	Total	C	N	O	S	0	0	0
			2514	1590	432	475	17			
1	O	305	Total	C	N	O	S	0	0	0
			2408	1527	413	452	16			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	GLY	-	EXPRESSION TAG	UNP P04526
B	-3	PRO	-	EXPRESSION TAG	UNP P04526
B	-2	GLY	-	EXPRESSION TAG	UNP P04526
B	-1	GLY	-	EXPRESSION TAG	UNP P04526
B	0	SER	-	EXPRESSION TAG	UNP P04526
C	-4	GLY	-	EXPRESSION TAG	UNP P04526
C	-3	PRO	-	EXPRESSION TAG	UNP P04526
C	-2	GLY	-	EXPRESSION TAG	UNP P04526
C	-1	GLY	-	EXPRESSION TAG	UNP P04526
C	0	SER	-	EXPRESSION TAG	UNP P04526
D	-4	GLY	-	EXPRESSION TAG	UNP P04526
D	-3	PRO	-	EXPRESSION TAG	UNP P04526
D	-2	GLY	-	EXPRESSION TAG	UNP P04526

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-1	GLY	-	EXPRESSION TAG	UNP P04526
D	0	SER	-	EXPRESSION TAG	UNP P04526
E	-4	GLY	-	EXPRESSION TAG	UNP P04526
E	-3	PRO	-	EXPRESSION TAG	UNP P04526
E	-2	GLY	-	EXPRESSION TAG	UNP P04526
E	-1	GLY	-	EXPRESSION TAG	UNP P04526
E	0	SER	-	EXPRESSION TAG	UNP P04526
L	-4	GLY	-	EXPRESSION TAG	UNP P04526
L	-3	PRO	-	EXPRESSION TAG	UNP P04526
L	-2	GLY	-	EXPRESSION TAG	UNP P04526
L	-1	GLY	-	EXPRESSION TAG	UNP P04526
L	0	SER	-	EXPRESSION TAG	UNP P04526
M	-4	GLY	-	EXPRESSION TAG	UNP P04526
M	-3	PRO	-	EXPRESSION TAG	UNP P04526
M	-2	GLY	-	EXPRESSION TAG	UNP P04526
M	-1	GLY	-	EXPRESSION TAG	UNP P04526
M	0	SER	-	EXPRESSION TAG	UNP P04526
N	-4	GLY	-	EXPRESSION TAG	UNP P04526
N	-3	PRO	-	EXPRESSION TAG	UNP P04526
N	-2	GLY	-	EXPRESSION TAG	UNP P04526
N	-1	GLY	-	EXPRESSION TAG	UNP P04526
N	0	SER	-	EXPRESSION TAG	UNP P04526
O	-4	GLY	-	EXPRESSION TAG	UNP P04526
O	-3	PRO	-	EXPRESSION TAG	UNP P04526
O	-2	GLY	-	EXPRESSION TAG	UNP P04526
O	-1	GLY	-	EXPRESSION TAG	UNP P04526
O	0	SER	-	EXPRESSION TAG	UNP P04526

- Molecule 2 is a protein called DNA polymerase accessory protein 62.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	186	Total	C	N	O	S	0	0	0
			1488	959	244	279	6			
2	K	186	Total	C	N	O	S	0	0	0
			1488	959	244	279	6			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	188	GLY	-	EXPRESSION TAG	UNP P04527
A	189	LEU	-	EXPRESSION TAG	UNP P04527
A	190	GLU	-	EXPRESSION TAG	UNP P04527

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Chain	Residue	Modelled	Actual	Comment	Reference
A	191	HIS	-	EXPRESSION TAG	UNP P04527
A	192	HIS	-	EXPRESSION TAG	UNP P04527
A	193	HIS	-	EXPRESSION TAG	UNP P04527
A	194	HIS	-	EXPRESSION TAG	UNP P04527
A	195	HIS	-	EXPRESSION TAG	UNP P04527
A	196	HIS	-	EXPRESSION TAG	UNP P04527
A	197	HIS	-	EXPRESSION TAG	UNP P04527
A	198	HIS	-	EXPRESSION TAG	UNP P04527
A	199	HIS	-	EXPRESSION TAG	UNP P04527
A	200	HIS	-	EXPRESSION TAG	UNP P04527
K	188	GLY	-	EXPRESSION TAG	UNP P04527
K	189	LEU	-	EXPRESSION TAG	UNP P04527
K	190	GLU	-	EXPRESSION TAG	UNP P04527
K	191	HIS	-	EXPRESSION TAG	UNP P04527
K	192	HIS	-	EXPRESSION TAG	UNP P04527
K	193	HIS	-	EXPRESSION TAG	UNP P04527
K	194	HIS	-	EXPRESSION TAG	UNP P04527
K	195	HIS	-	EXPRESSION TAG	UNP P04527
K	196	HIS	-	EXPRESSION TAG	UNP P04527
K	197	HIS	-	EXPRESSION TAG	UNP P04527
K	198	HIS	-	EXPRESSION TAG	UNP P04527
K	199	HIS	-	EXPRESSION TAG	UNP P04527
K	200	HIS	-	EXPRESSION TAG	UNP P04527

- Molecule 3 is a protein called DNA polymerase processivity component.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	228	Total	C	N	O	Se	0	0	0
			1750	1113	288	343	6			
3	H	228	Total	C	N	O	Se	0	0	0
			1750	1113	288	343	6			
3	F	228	Total	C	N	O	Se	0	0	0
			1750	1113	288	343	6			
3	Q	228	Total	C	N	O	Se	0	0	0
			1750	1113	288	343	6			
3	R	228	Total	C	N	O	Se	0	0	0
			1750	1113	288	343	6			
3	P	228	Total	C	N	O	Se	0	0	0
			1750	1113	288	343	6			

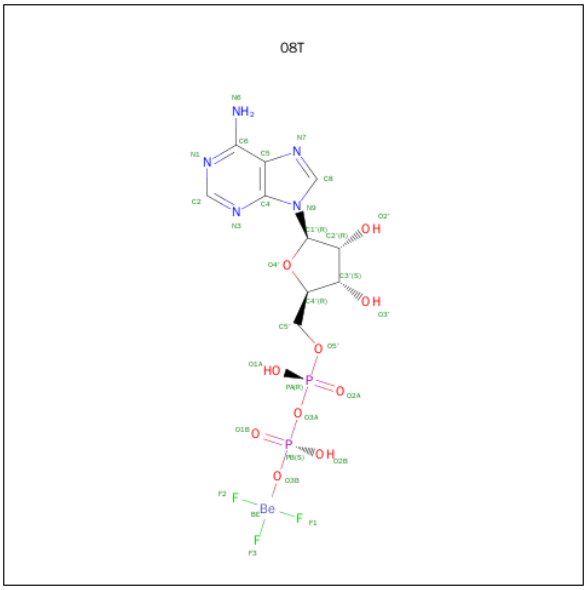
- Molecule 4 is a DNA chain called Template DNA strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	I	24	Total	C	N	O	P	0	0	0
			489	236	76	153	24			
4	S	24	Total	C	N	O	P	0	0	0
			489	236	76	153	24			

- Molecule 5 is a DNA chain called Primer DNA strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	J	20	Total	C	N	O	P	0	0	0
			411	195	81	115	20			
5	T	20	Total	C	N	O	P	0	0	0
			411	195	81	115	20			

- Molecule 6 is [[[(2R,3S,4R,5R)-5-(6-AMINOPURIN-9-YL)-3,4-BIS(OXIDANYL)OXOLAN-2-YL]METHOXY-OXIDANYL-PHOSPHORYL]OXY-OXIDANYL-PHOSPHORYL]OXY-TRIS(FLUORANYL)BERYLLIUM (three-letter code: 08T) (formula: $C_{10}H_{14}BeF_3N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
6	B	1	Total	Be	C	F	N	O	P	0	0
			31	1	10	3	5	10	2		
6	C	1	Total	Be	C	F	N	O	P	0	0
			31	1	10	3	5	10	2		
6	D	1	Total	Be	C	F	N	O	P	0	0
			31	1	10	3	5	10	2		
6	L	1	Total	Be	C	F	N	O	P	0	0
			31	1	10	3	5	10	2		

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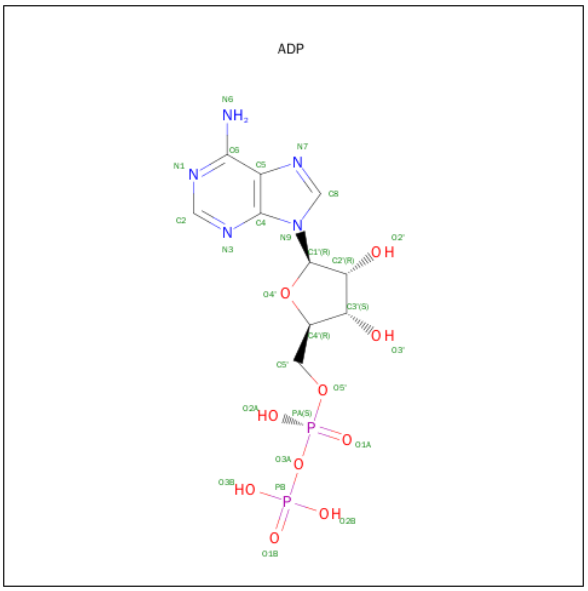
Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
6	M	1	Total	Be	C	F	N	O	P	0	0
			31	1	10	3	5	10	2		
6	N	1	Total	Be	C	F	N	O	P	0	0
			31	1	10	3	5	10	2		

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	D	1	Total	Mg	0	0
			1	1		
7	E	1	Total	Mg	0	0
			1	1		
7	B	1	Total	Mg	0	0
			1	1		
7	C	1	Total	Mg	0	0
			1	1		
7	N	1	Total	Mg	0	0
			1	1		
7	O	1	Total	Mg	0	0
			1	1		
7	L	1	Total	Mg	0	0
			1	1		
7	M	1	Total	Mg	0	0
			1	1		

- Molecule 8 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



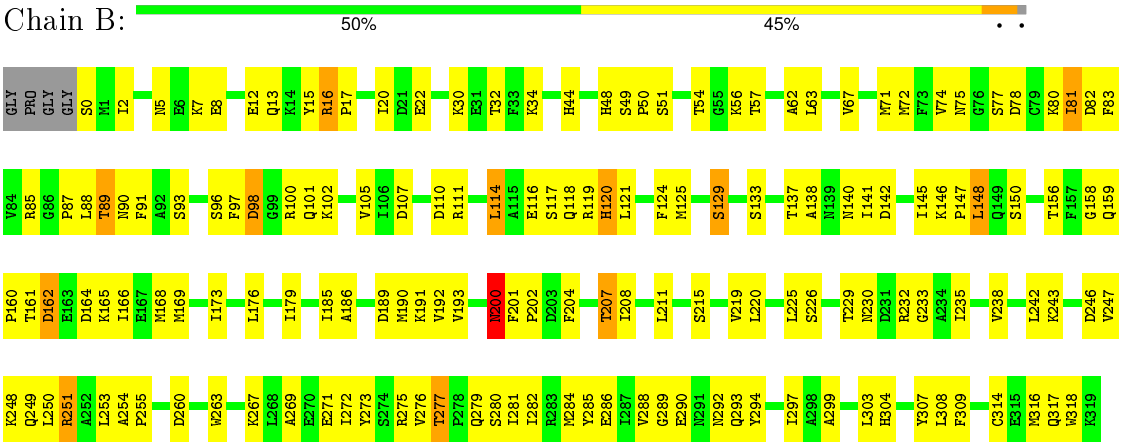
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
8	O	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

3 Residue-property plots (i)

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

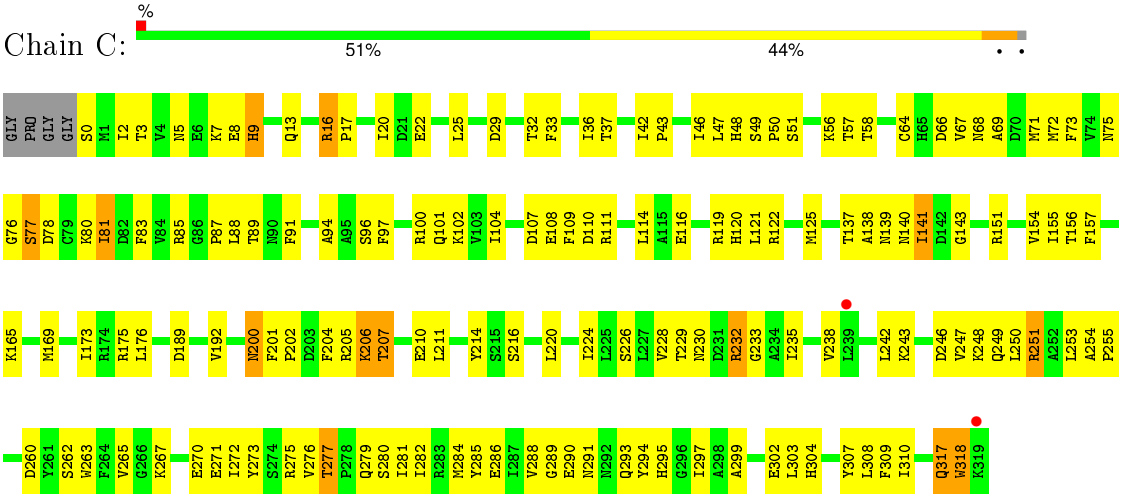
- Molecule 1: DNA polymerase accessory protein 44

Chain B:



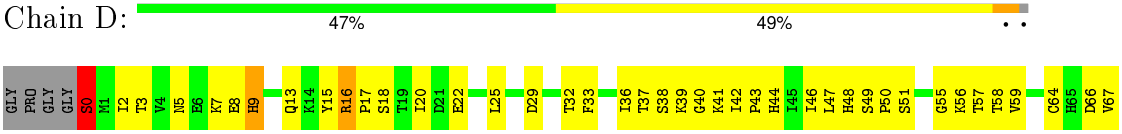
- Molecule 1: DNA polymerase accessory protein 44

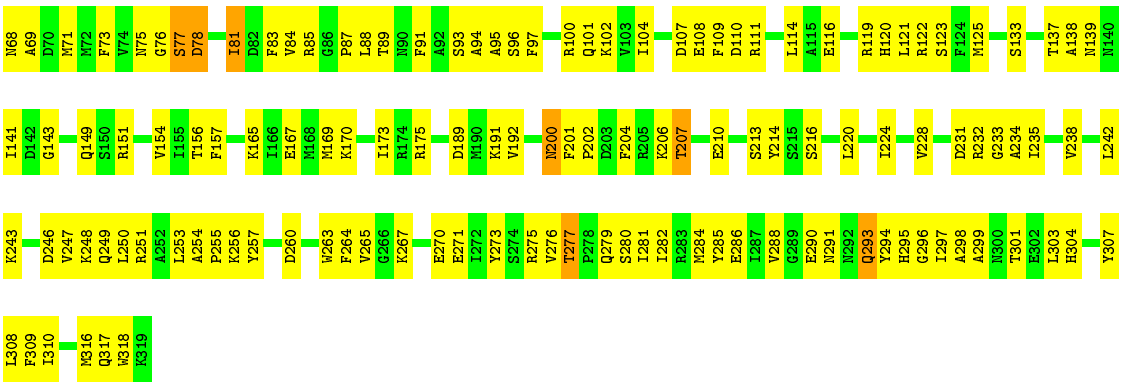
Chain C:



- Molecule 1: DNA polymerase accessory protein 44

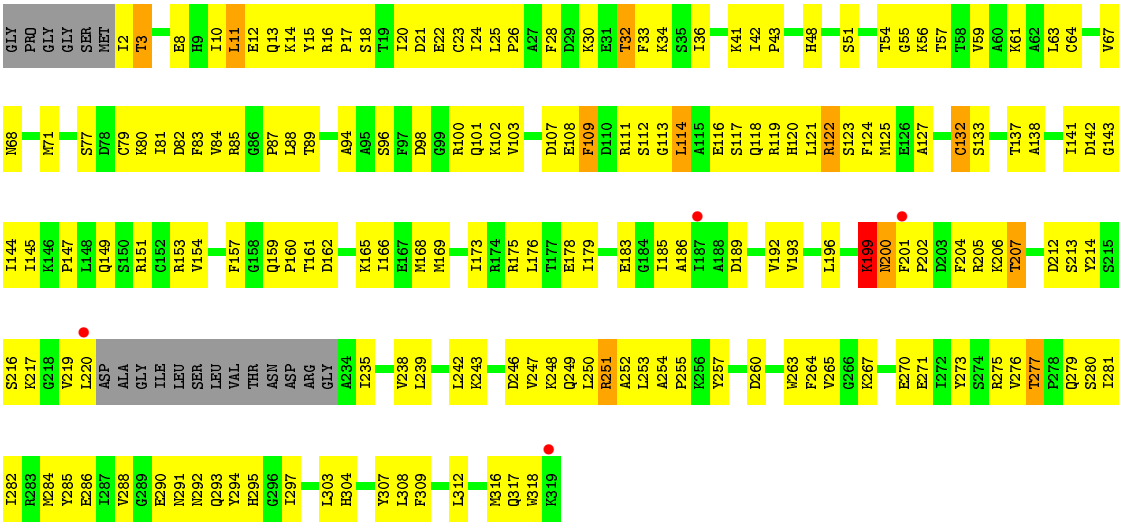
Chain D:





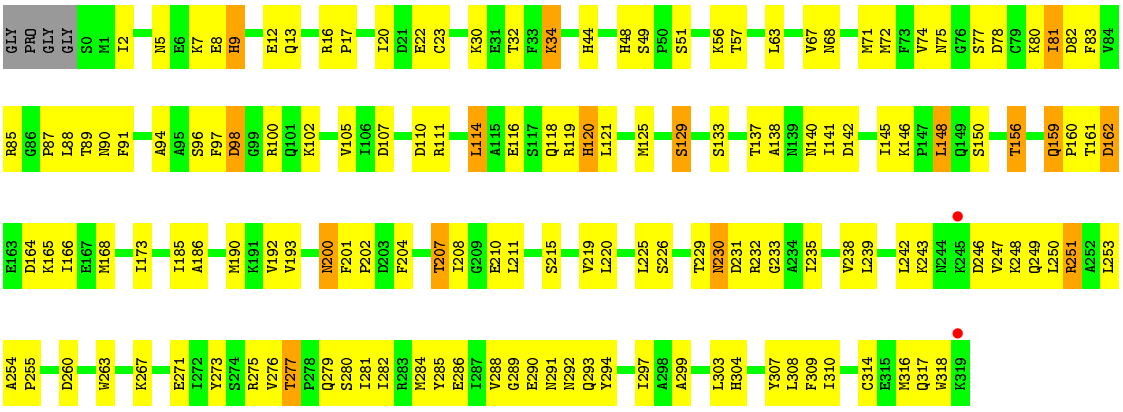
• Molecule 1: DNA polymerase accessory protein 44

Chain E:



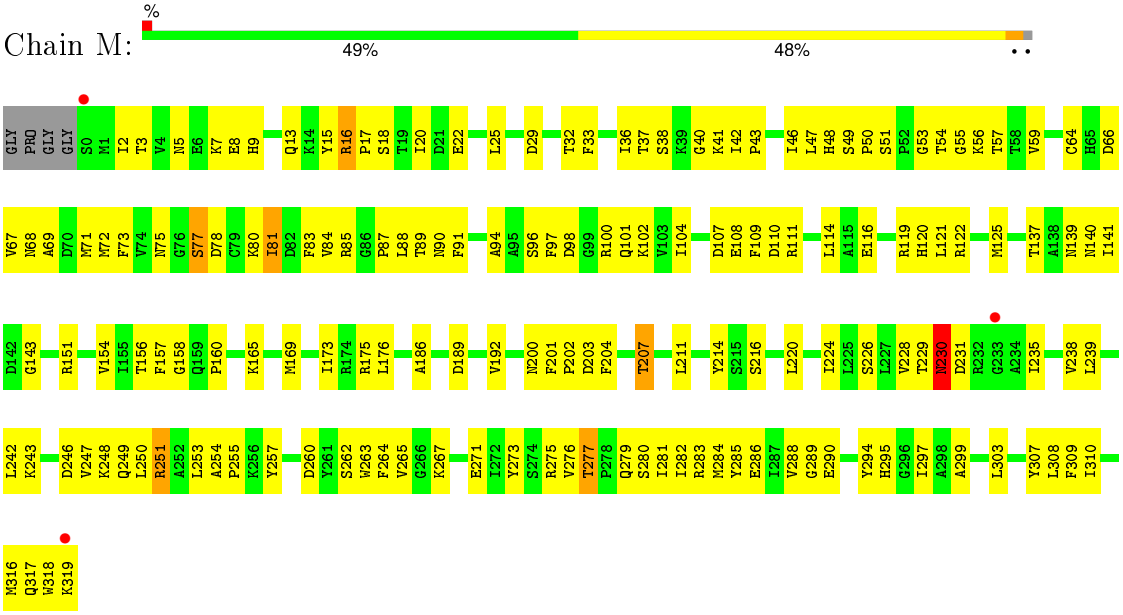
• Molecule 1: DNA polymerase accessory protein 44

Chain L:



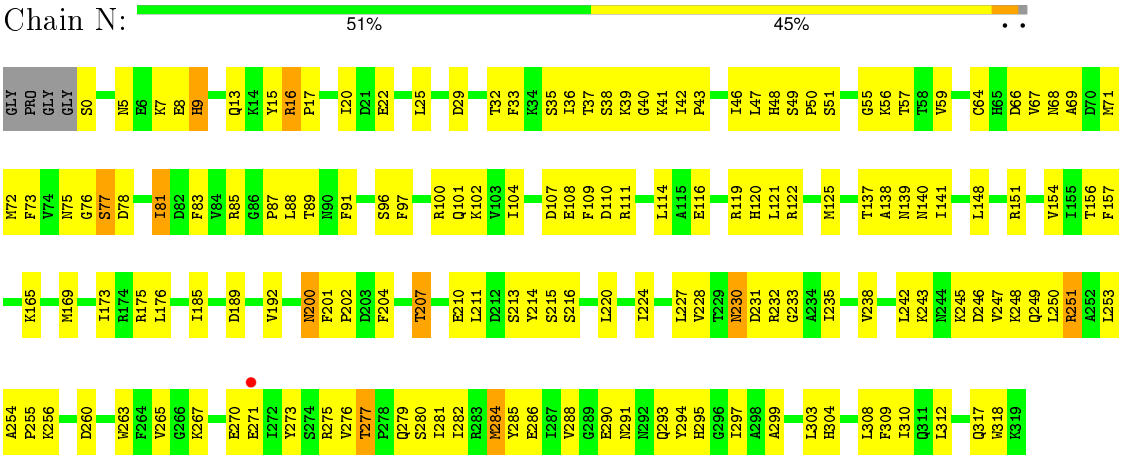
• Molecule 1: DNA polymerase accessory protein 44

Chain M:



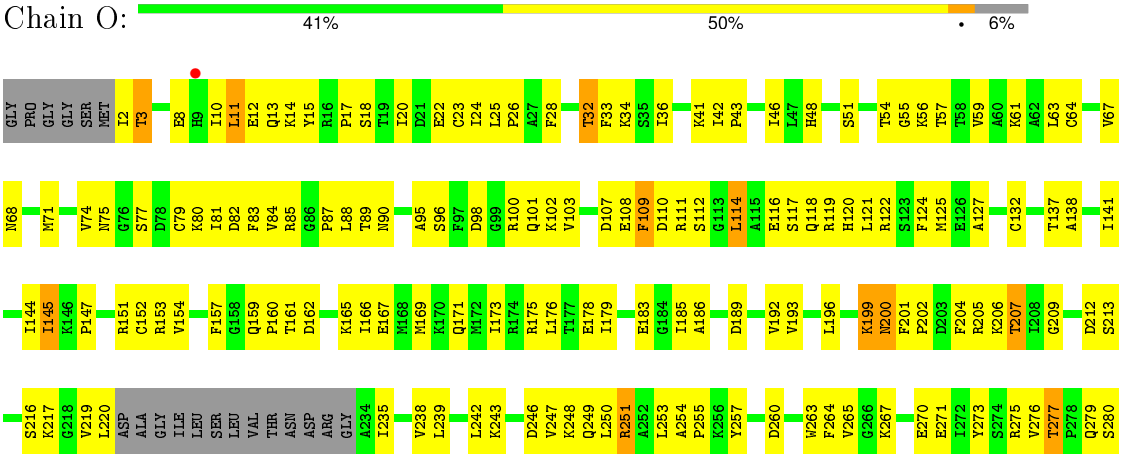
• Molecule 1: DNA polymerase accessory protein 44

Chain N:



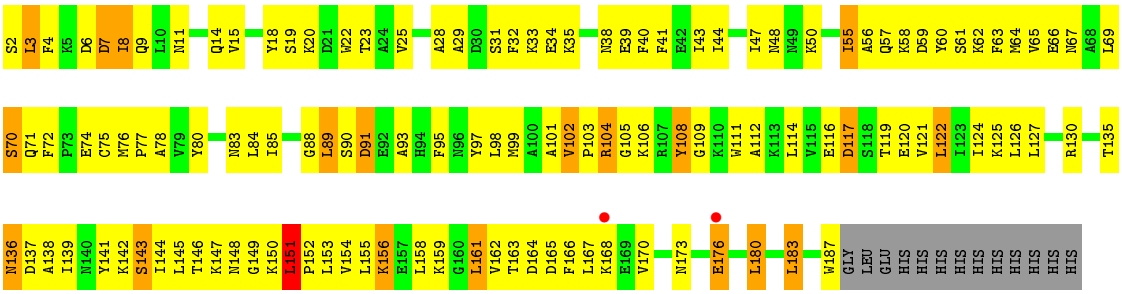
• Molecule 1: DNA polymerase accessory protein 44

Chain O:



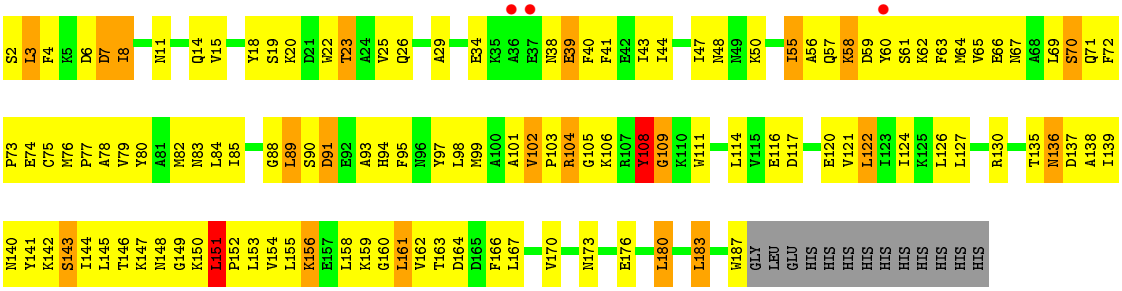
• Molecule 2: DNA polymerase accessory protein 62

Chain A:



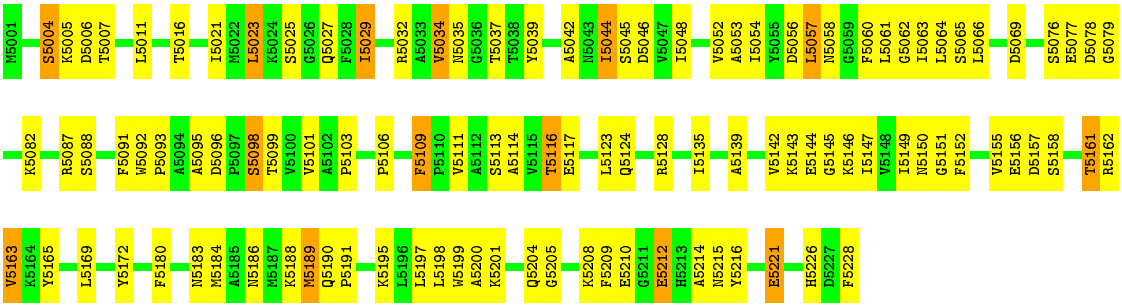
• Molecule 2: DNA polymerase accessory protein 62

Chain K:



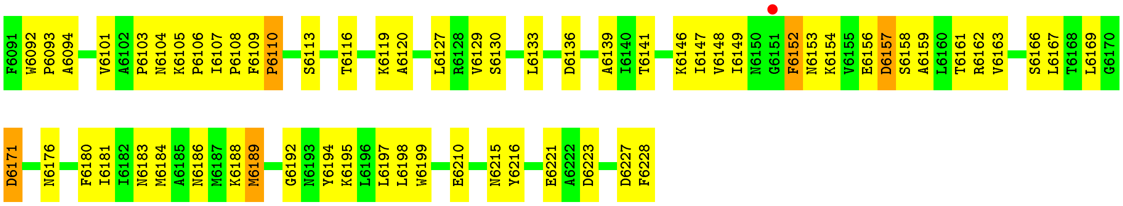
• Molecule 3: DNA polymerase processivity component

Chain G:



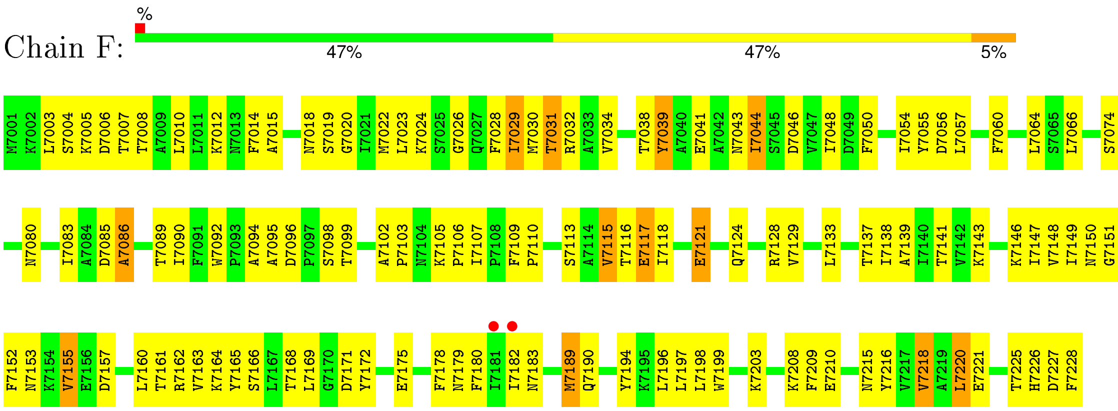
• Molecule 3: DNA polymerase processivity component

Chain H:



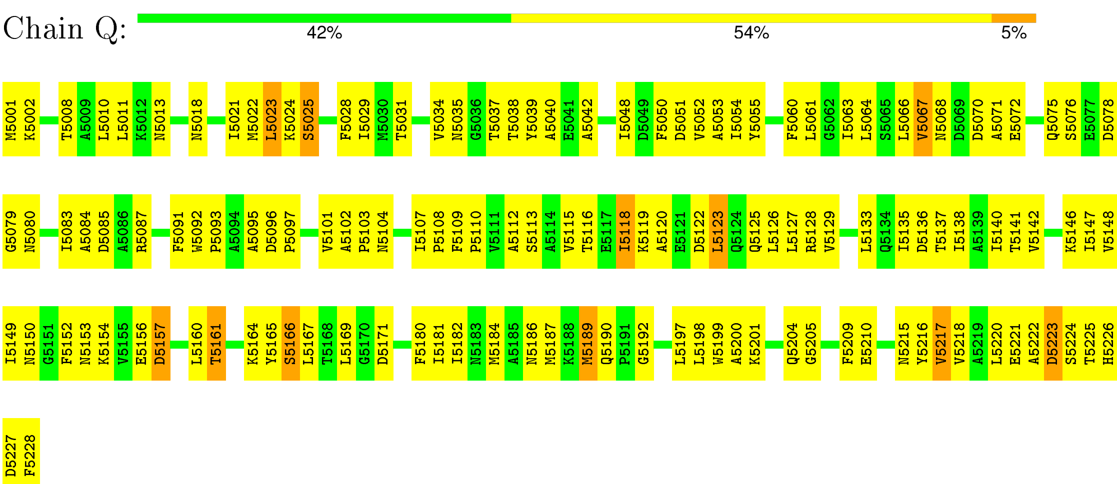
- Molecule 3: DNA polymerase processivity component

Chain F:



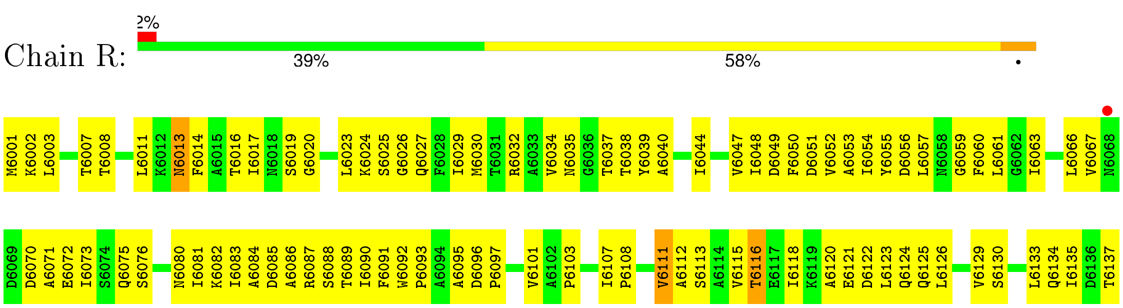
- Molecule 3: DNA polymerase processivity component

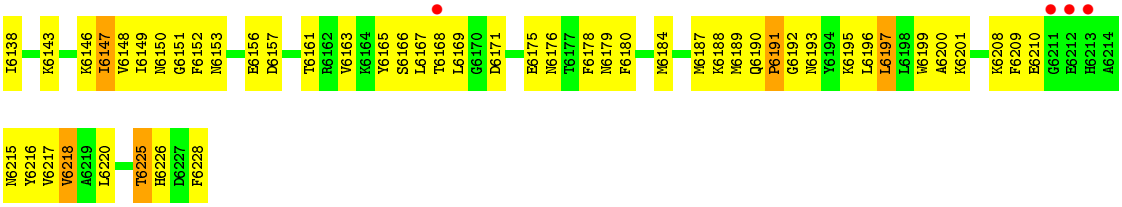
Chain Q:



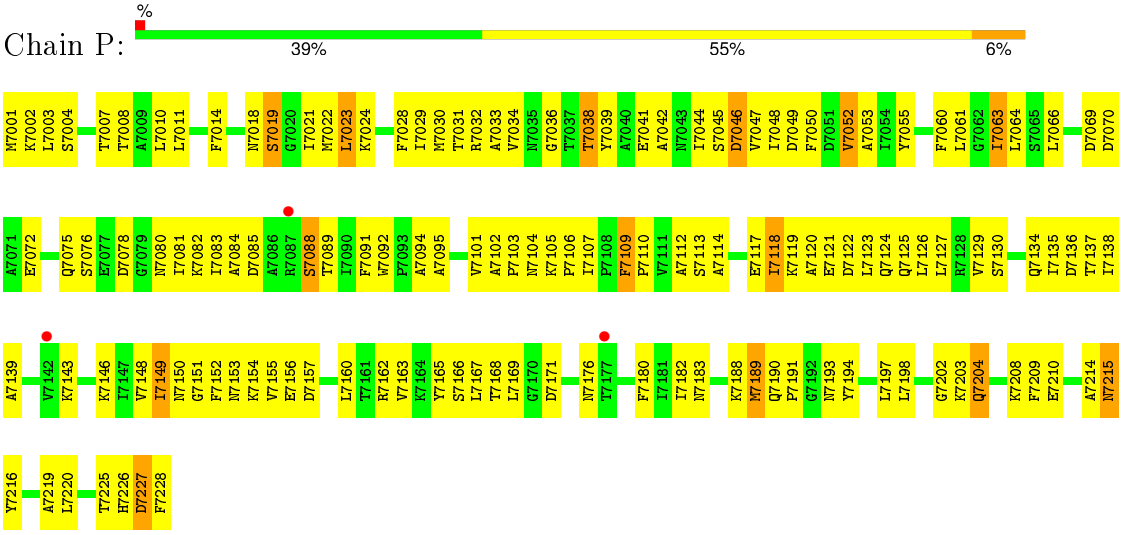
- Molecule 3: DNA polymerase processivity component

Chain R:

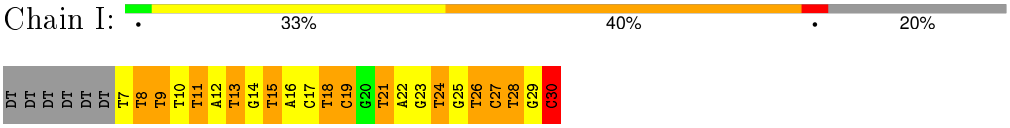




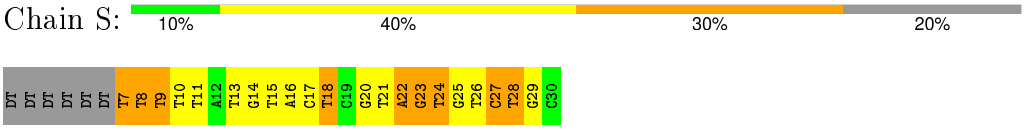
• Molecule 3: DNA polymerase processivity component



• Molecule 4: Template DNA strand

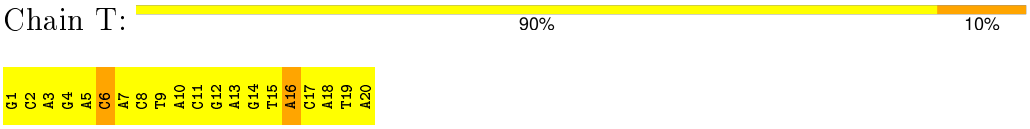


• Molecule 4: Template DNA strand



• Molecule 5: Primer DNA strand

• Molecule 5: Primer DNA strand



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	95.70Å 239.18Å 247.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.19 – 3.50 49.19 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.3 (49.19-3.50) 99.3 (49.19-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.16	Depositor
$< I/\sigma(I) >$ [1]	3.00 (at 3.48Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.231 , 0.279 0.228 , 0.275	Depositor DCC
R_{free} test set	1985 reflections (2.83%)	DCC
Wilson B-factor (Å^2)	77.3	Xtriage
Anisotropy	0.404	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 65.3	EDS
Estimated twinning fraction	0.003 for -h,l,k	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.30$	Xtriage
Outliers	0 of 72021 reflections	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	35424	wwPDB-VP
Average B, all atoms (Å^2)	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.95% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ADP, 08T

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	B	0.63	1/2558 (0.0%)	0.77	0/3449
1	C	0.64	0/2558	0.77	4/3449 (0.1%)
1	D	0.64	1/2558 (0.0%)	0.75	0/3449
1	E	0.56	0/2451	0.71	0/3303
1	L	0.60	2/2558 (0.1%)	0.73	0/3449
1	M	0.64	0/2558	0.76	1/3449 (0.0%)
1	N	0.60	0/2558	0.75	0/3449
1	O	0.55	0/2451	0.71	0/3303
2	A	0.51	0/1516	0.74	1/2042 (0.0%)
2	K	0.48	0/1516	0.74	2/2042 (0.1%)
3	F	0.48	0/1774	0.71	0/2395
3	G	0.53	0/1774	0.73	0/2395
3	H	0.51	0/1774	0.70	0/2395
3	P	0.51	0/1774	0.75	0/2395
3	Q	0.56	0/1774	0.78	0/2395
3	R	0.59	0/1774	0.78	1/2395 (0.0%)
4	I	6.29	1/544 (0.2%)	3.85	28/838 (3.3%)
4	S	1.16	1/544 (0.2%)	1.91	19/838 (2.3%)
5	J	0.92	0/462	1.72	11/710 (1.5%)
5	T	0.90	0/462	1.53	2/710 (0.3%)
All	All	0.98	6/35938 (0.0%)	0.95	69/48850 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	C	0	1
1	D	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	L	0	2
1	M	0	2
1	N	0	2
2	A	0	1
2	K	0	2
4	I	0	1
All	All	0	13

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	30	DC	C1'-N1	144.35	3.49	1.47
4	S	15	DT	N1-C2	6.50	1.43	1.38
1	B	159	GLN	CD-NE2	-6.26	1.17	1.32
1	L	159	GLN	CD-NE2	-6.05	1.17	1.32
1	D	293	GLN	CD-NE2	5.66	1.47	1.32
1	L	159	GLN	CD-OE1	-5.54	1.11	1.24

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	I	30	DC	O4'-C1'-N1	-87.18	46.97	108.00
4	I	30	DC	C2-N1-C1'	-30.76	84.97	118.80
4	I	30	DC	C6-N1-C1'	18.13	142.56	120.80
4	S	15	DT	N3-C2-O2	-9.38	116.67	122.30
5	J	16	DA	O4'-C1'-N9	9.33	114.53	108.00
5	J	15	DT	O4'-C1'-N1	9.09	114.36	108.00
4	I	15	DT	N3-C2-O2	-9.04	116.87	122.30
4	I	28	DT	O4'-C1'-N1	8.05	113.64	108.00
5	T	6	DC	O4'-C1'-N1	7.72	113.40	108.00
4	I	11	DT	N3-C4-O4	7.71	124.53	119.90
4	I	13	DT	N3-C4-O4	7.63	124.48	119.90
4	I	27	DC	O4'-C1'-N1	7.26	113.08	108.00
5	J	2	DC	O4'-C1'-N1	7.15	113.01	108.00
4	S	22	DA	O4'-C1'-N9	7.07	112.95	108.00
5	J	6	DC	O4'-C1'-N1	7.03	112.92	108.00
4	I	8	DT	O4'-C1'-N1	-7.01	103.09	108.00
4	S	15	DT	O4'-C1'-C2'	-6.83	100.43	105.90
4	I	18	DT	O4'-C1'-N1	6.76	112.73	108.00
4	S	15	DT	N1-C2-O2	6.72	128.48	123.10
4	I	26	DT	O4'-C1'-N1	6.54	112.58	108.00
4	I	24	DT	C5-C4-O4	-6.47	120.37	124.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	I	15	DT	N3-C4-O4	6.42	123.75	119.90
4	I	9	DT	C4-C5-C7	6.30	122.78	119.00
1	M	230	ASN	CA-C-N	-6.24	103.47	117.20
4	I	9	DT	C6-C5-C7	-6.22	119.17	122.90
4	S	24	DT	C6-C5-C7	-6.22	119.17	122.90
4	S	24	DT	C4-C5-C7	6.13	122.68	119.00
5	J	14	DG	C6-C5-N7	-6.07	126.76	130.40
4	I	15	DT	N1-C2-O2	6.06	127.95	123.10
4	I	24	DT	N3-C4-O4	6.02	123.51	119.90
4	S	27	DC	O4'-C1'-N1	5.98	112.19	108.00
4	S	15	DT	O4'-C1'-N1	5.92	112.14	108.00
1	C	233	GLY	N-CA-C	5.88	127.79	113.10
4	S	11	DT	O4'-C1'-C2'	5.79	110.53	105.90
4	S	18	DT	N3-C2-O2	-5.78	118.83	122.30
4	I	7	DT	C5-C4-O4	-5.76	120.87	124.90
4	S	7	DT	C5-C4-O4	-5.76	120.87	124.90
4	S	21	DT	O4'-C1'-N1	-5.70	104.01	108.00
4	S	9	DT	N3-C2-O2	-5.64	118.92	122.30
2	A	117	ASP	N-CA-C	-5.62	95.84	111.00
3	R	6026	GLY	N-CA-C	-5.59	99.12	113.10
5	J	1	DG	N1-C6-O6	5.53	123.22	119.90
5	J	14	DG	N1-C6-O6	5.51	123.21	119.90
5	T	16	DA	N1-C6-N6	5.50	121.90	118.60
4	S	18	DT	O4'-C1'-N1	5.48	111.84	108.00
4	S	27	DC	C1'-O4'-C4'	-5.48	104.62	110.10
2	K	117	ASP	N-CA-C	-5.45	96.30	111.00
4	I	21	DT	C5-C4-O4	-5.43	121.10	124.90
4	S	13	DT	O4'-C1'-N1	5.38	111.77	108.00
4	I	19	DC	O4'-C4'-C3'	5.37	109.22	106.00
4	I	11	DT	C5-C4-O4	-5.36	121.14	124.90
4	I	9	DT	N3-C2-O2	-5.34	119.09	122.30
4	I	21	DT	N3-C4-O4	5.33	123.10	119.90
4	I	7	DT	N3-C4-O4	5.32	123.09	119.90
5	J	9	DT	C5-C4-O4	-5.31	121.18	124.90
5	J	12	DG	C8-N9-C4	-5.25	104.30	106.40
5	J	18	DA	C4'-C3'-C2'	-5.25	98.37	103.10
4	S	8	DT	C5-C4-O4	-5.20	121.26	124.90
4	S	23	DG	O4'-C1'-N9	5.19	111.63	108.00
1	C	141	ILE	CB-CA-C	-5.12	101.35	111.60
2	K	108	TYR	N-CA-C	-5.12	97.18	111.00
4	I	28	DT	C5-C4-O4	-5.07	121.35	124.90
4	S	28	DT	N3-C4-O4	5.04	122.92	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	233	GLY	C-N-CA	5.04	134.29	121.70
4	I	13	DT	C5-C4-O4	-5.03	121.38	124.90
4	I	7	DT	O4'-C1'-N1	-5.03	104.48	108.00
1	C	206	LYS	CD-CE-NZ	5.02	123.25	111.70
5	J	14	DG	C4-C5-C6	5.01	121.81	118.80
4	I	15	DT	O4'-C1'-N1	5.00	111.50	108.00

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	7	ASP	Mainchain
1	B	200	ASN	Peptide
1	C	229	THR	Peptide
1	D	0	SER	Peptide
4	I	30	DC	Sidechain
2	K	109	GLY	Peptide
2	K	7	ASP	Mainchain
1	L	200	ASN	Peptide
1	L	230	ASN	Peptide
1	M	229	THR	Peptide
1	M	230	ASN	Peptide
1	N	230	ASN	Peptide
1	N	233	GLY	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2514	0	2543	178	0
1	C	2514	0	2543	192	0
1	D	2514	0	2543	251	0
1	E	2408	0	2433	221	0
1	L	2514	0	2543	167	0
1	M	2514	0	2543	188	0
1	N	2514	0	2543	215	0
1	O	2408	0	2433	215	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	1488	0	1509	173	0
2	K	1488	0	1509	184	0
3	F	1750	0	1752	117	0
3	G	1750	0	1752	140	0
3	H	1750	0	1752	95	0
3	P	1750	0	1752	182	0
3	Q	1750	0	1752	138	0
3	R	1750	0	1752	164	0
4	I	489	0	277	43	0
4	S	489	0	277	37	0
5	J	411	0	224	31	0
5	T	411	0	224	27	0
6	B	31	0	13	8	0
6	C	31	0	13	8	0
6	D	31	0	13	6	0
6	L	31	0	13	6	0
6	M	31	0	13	9	0
6	N	31	0	13	7	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
7	E	1	0	0	0	0
7	L	1	0	0	0	0
7	M	1	0	0	0	0
7	N	1	0	0	0	0
7	O	1	0	0	0	0
8	E	27	0	12	5	0
8	O	27	0	12	4	0
All	All	35424	0	34758	2554	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 36.

All (2554) 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)
1:L:293:GLN:NE2	2:K:84:LEU:O	1.73	1.21
1:N:108:GLU:HB3	1:O:122:ARG:HH21	1.06	1.19
3:P:7109:PHE:HD1	3:P:7110:PRO:HD2	1.02	1.18
3:Q:5128:ARG:HG2	3:P:7066:LEU:HD13	1.24	1.13
3:F:7141:THR:HG22	3:F:7179:ASN:HA	1.26	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:111:ARG:HG2	1:E:112:SER:N	1.60	1.12
1:M:297:ILE:HD13	1:N:297:ILE:HD11	1.32	1.12
1:B:293:GLN:NE2	2:A:84:LEU:O	1.85	1.10
2:A:164:ASP:HA	2:A:167:LEU:HD12	1.27	1.10
2:K:164:ASP:HA	2:K:167:LEU:HD12	1.23	1.10
1:L:248:LYS:HG2	1:M:273:TYR:OH	1.50	1.09
1:O:111:ARG:HG2	1:O:112:SER:N	1.65	1.08
1:D:276:VAL:HG23	1:D:318:TRP:HB3	1.33	1.07
3:P:7109:PHE:CD1	3:P:7110:PRO:HD2	1.90	1.07
1:L:56:LYS:NZ	6:L:700:08T:O2B	1.86	1.06
1:N:77:SER:HB3	1:N:111:ARG:HH11	1.19	1.06
1:L:77:SER:HB3	1:L:111:ARG:HH11	1.21	1.05
1:L:314:CYS:SG	1:M:282:ILE:HD11	1.96	1.05
1:B:77:SER:HB3	1:B:111:ARG:HH11	1.16	1.05
1:C:297:ILE:HD13	1:D:297:ILE:HD11	1.38	1.05
1:D:77:SER:HB3	1:D:111:ARG:HH11	1.18	1.04
1:E:111:ARG:NH2	4:I:13:DT:OP1	1.90	1.04
1:O:111:ARG:HG2	1:O:112:SER:H	0.89	1.04
1:B:248:LYS:HG2	1:C:273:TYR:OH	1.57	1.03
2:K:55:ILE:HG12	2:K:56:ALA:H	1.23	1.02
1:O:111:ARG:HB3	1:O:114:LEU:HD22	1.42	1.01
1:M:77:SER:HB3	1:M:111:ARG:HH11	1.22	1.01
2:K:155:LEU:HD22	2:K:183:LEU:HD21	1.42	1.01
3:Q:5076:SER:HG	3:Q:5091:PHE:HE1	1.09	1.01
1:N:256:LYS:HE3	1:O:159:GLN:NE2	1.75	1.00
3:G:5087:ARG:HH12	3:H:6119:LYS:HD2	1.26	1.00
3:G:5135:ILE:HD13	3:G:5151:GLY:HA3	1.40	1.00
6:M:700:08T:N3	6:M:700:08T:H6	1.76	1.00
1:L:12:GLU:O	6:L:700:08T:O3'	1.80	1.00
3:F:7080:ASN:HA	3:F:7094:ALA:HB2	1.42	1.00
1:O:251:ARG:NH1	2:K:70:SER:OG	1.92	1.00
1:C:48:HIS:CE1	1:C:141:ILE:HD11	1.96	1.00
1:D:16:ARG:NH2	6:D:700:08T:O2A	1.95	0.99
1:N:297:ILE:HD13	1:O:297:ILE:HD11	1.41	0.99
1:D:48:HIS:CE1	1:D:141:ILE:HD11	1.98	0.99
1:E:111:ARG:HG2	1:E:112:SER:H	0.85	0.98
1:C:165:LYS:HG2	1:C:169:MET:HE2	1.43	0.98
1:O:145:ILE:HG13	1:O:147:PRO:HD2	1.42	0.98
1:L:97:PHE:CZ	3:P:7078:ASP:HB2	1.98	0.98
3:Q:5210:GLU:HA	3:Q:5215:ASN:ND2	1.76	0.98
3:H:6180:PHE:HD2	3:H:6198:LEU:HD13	1.24	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:111:ARG:HB3	1:E:114:LEU:HD22	1.43	0.97
1:N:299:ALA:HB2	1:O:295:HIS:HD2	1.25	0.97
1:M:97:PHE:O	3:Q:5204:GLN:HA	1.64	0.97
3:F:7133:LEU:O	3:F:7164:LYS:NZ	1.97	0.97
1:E:316:MET:HB3	1:E:318:TRP:HZ3	1.29	0.97
1:L:299:ALA:HB1	1:M:262:SER:HB3	1.46	0.97
1:M:48:HIS:CE1	1:M:141:ILE:HD11	1.99	0.96
2:K:47:ILE:O	2:K:50:LYS:NZ	1.99	0.95
1:D:108:GLU:HB3	1:E:122:ARG:HH21	1.31	0.95
3:Q:5038:THR:HG21	3:Q:5186:ASN:O	1.66	0.95
1:N:48:HIS:CE1	1:N:141:ILE:HD11	2.01	0.95
1:C:77:SER:HB3	1:C:111:ARG:HH11	1.28	0.95
1:C:303:LEU:HD22	1:D:265:VAL:CG1	1.97	0.95
1:E:111:ARG:CG	1:E:112:SER:H	1.76	0.95
1:L:9:HIS:CD2	1:M:41:LYS:HB3	2.02	0.95
3:P:7007:THR:HG23	3:P:7044:ILE:HG12	1.49	0.95
2:A:7:ASP:OD2	3:F:7032:ARG:NH1	2.00	0.95
1:D:251:ARG:NH2	1:E:270:GLU:HA	1.82	0.94
3:F:7056:ASP:HB3	3:F:7092:TRP:HZ2	1.32	0.94
1:N:77:SER:HB2	1:O:120:HIS:HD2	1.32	0.94
1:B:48:HIS:CE1	1:B:141:ILE:HD11	2.03	0.94
2:A:55:ILE:HG12	2:A:56:ALA:H	1.28	0.94
3:F:7148:VAL:HG12	3:F:7168:THR:HA	1.50	0.94
1:N:276:VAL:HG23	1:N:318:TRP:HB3	1.50	0.93
1:C:251:ARG:HH21	1:D:270:GLU:HG3	1.33	0.93
3:P:7109:PHE:HD1	3:P:7110:PRO:CD	1.80	0.93
2:K:7:ASP:OD2	3:P:7032:ARG:NH1	2.01	0.93
2:A:47:ILE:O	2:A:50:LYS:NZ	2.02	0.93
1:O:212:ASP:HB3	2:K:144:ILE:HG21	1.51	0.93
1:E:277:THR:HG22	1:E:317:GLN:O	1.67	0.93
1:E:145:ILE:HG13	1:E:147:PRO:HD2	1.51	0.93
1:N:9:HIS:HD2	1:O:41:LYS:HB3	1.30	0.93
1:M:310:ILE:HG12	1:N:285:TYR:HD2	1.33	0.92
2:A:155:LEU:HD22	2:A:183:LEU:HD21	1.50	0.92
1:E:186:ALA:HB3	1:E:219:VAL:HG22	1.50	0.92
1:N:88:LEU:HD22	1:N:104:ILE:HD13	1.51	0.92
1:D:57:THR:HG22	1:D:107:ASP:OD1	1.69	0.92
3:R:6146:LYS:HA	3:R:6171:ASP:HA	1.52	0.92
4:I:17:DC:N3	5:J:14:DG:N2	2.18	0.92
1:O:251:ARG:HE	2:K:71:GLN:CD	1.73	0.92
1:O:186:ALA:HB3	1:O:219:VAL:HG22	1.51	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:S:14:DG:N2	5:T:17:DC:O2	2.03	0.92
1:N:256:LYS:HE3	1:O:159:GLN:HE21	1.33	0.91
3:F:7161:THR:HG23	3:F:7162:ARG:HG3	1.50	0.91
1:O:111:ARG:CG	1:O:112:SER:H	1.81	0.91
1:C:299:ALA:HB2	1:D:295:HIS:HD2	1.35	0.91
1:E:251:ARG:HE	2:A:71:GLN:CD	1.74	0.91
1:O:277:THR:HG22	1:O:317:GLN:O	1.71	0.91
1:D:297:ILE:HD13	1:E:297:ILE:HD11	1.50	0.91
1:N:9:HIS:CD2	1:O:41:LYS:HB3	2.06	0.91
3:Q:5128:ARG:HD3	3:P:7066:LEU:HD22	1.50	0.90
1:C:9:HIS:CD2	1:D:41:LYS:HB3	2.05	0.90
1:C:57:THR:HG22	1:C:107:ASP:OD1	1.69	0.90
1:B:81:ILE:HD11	1:B:120:HIS:CD2	2.06	0.90
2:K:3:LEU:HD21	3:P:7219:ALA:HB2	1.53	0.90
3:H:6149:ILE:HD12	3:H:6167:LEU:HD23	1.53	0.90
3:H:6030:MSE:HG3	3:H:6103:PRO:HG3	1.54	0.89
1:N:256:LYS:CE	1:O:159:GLN:NE2	2.35	0.89
1:D:277:THR:HG22	1:D:317:GLN:O	1.72	0.89
3:P:7118:ILE:HG12	3:P:7119:LYS:N	1.84	0.89
1:L:97:PHE:CE2	3:P:7078:ASP:HB2	2.06	0.89
1:E:2:ILE:HD12	1:E:178:GLU:HG2	1.54	0.89
1:B:299:ALA:HB1	1:C:262:SER:HB3	1.52	0.89
1:N:49:SER:HB3	1:N:56:LYS:NZ	1.88	0.89
1:L:48:HIS:CE1	1:L:141:ILE:HD11	2.07	0.89
3:P:7109:PHE:HD2	3:P:7208:LYS:HD3	1.38	0.88
1:D:49:SER:HB3	1:D:56:LYS:NZ	1.88	0.88
1:E:251:ARG:NH1	2:A:70:SER:OG	2.05	0.88
1:N:57:THR:HG22	1:N:107:ASP:OD1	1.73	0.88
1:B:260:ASP:OD2	1:C:50:PRO:HG2	1.73	0.88
1:D:299:ALA:HB2	1:E:295:HIS:HD2	1.37	0.88
3:P:7033:ALA:HB2	3:P:7038:THR:HG23	1.53	0.88
1:B:314:CYS:SG	1:C:282:ILE:HD11	2.14	0.88
1:N:108:GLU:HB3	1:O:122:ARG:NH2	1.87	0.88
1:N:251:ARG:NH2	1:O:270:GLU:HA	1.87	0.88
3:F:7141:THR:CG2	3:F:7179:ASN:HA	2.04	0.88
1:N:243:LYS:HE2	1:N:318:TRP:HE1	1.39	0.88
1:C:49:SER:HB3	1:C:56:LYS:NZ	1.88	0.88
1:N:299:ALA:HB2	1:O:295:HIS:CD2	2.09	0.88
3:G:5053:ALA:HB3	3:G:5095:ALA:O	1.74	0.87
1:M:57:THR:HG22	1:M:107:ASP:OD1	1.73	0.87
3:Q:5210:GLU:HA	3:Q:5215:ASN:HD22	1.35	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:246:ASP:OD2	1:M:249:GLN:HG3	1.75	0.87
3:G:5189:MSE:HB2	3:G:5216:TYR:CE2	2.09	0.86
1:D:9:HIS:CD2	1:E:41:LYS:HB3	2.11	0.86
3:G:5156:GLU:HG2	3:G:5162:ARG:HH21	1.40	0.86
3:H:6113:SER:HB2	3:H:6199:TRP:HA	1.58	0.86
1:O:176:LEU:HA	1:O:179:ILE:HD12	1.56	0.86
3:G:5210:GLU:HA	3:G:5215:ASN:HD22	1.39	0.86
2:K:90:SER:HB3	2:K:93:ALA:H	1.40	0.86
1:N:77:SER:HB2	1:O:120:HIS:CD2	2.10	0.86
1:C:232:ARG:CZ	1:C:260:ASP:OD2	2.24	0.86
1:B:77:SER:HB3	1:B:111:ARG:NH1	1.91	0.86
1:L:9:HIS:HD2	1:M:41:LYS:CB	1.88	0.86
3:P:7146:LYS:HG2	3:P:7171:ASP:HB3	1.58	0.86
3:G:5087:ARG:NH1	3:H:6119:LYS:HD2	1.90	0.85
1:C:58:THR:HG1	6:C:700:08T:H9	1.19	0.85
1:N:72:MET:HE2	3:R:6156:GLU:HA	1.56	0.85
1:D:170:LYS:HZ1	1:N:39:LYS:N	1.74	0.85
1:M:276:VAL:HG23	1:M:318:TRP:HB3	1.57	0.85
5:T:1:DG:H2"	5:T:2:DC:OP2	1.76	0.85
1:D:77:SER:HB2	1:E:120:HIS:HD2	1.39	0.85
1:M:49:SER:HB3	1:M:56:LYS:NZ	1.90	0.85
1:E:316:MET:HB3	1:E:318:TRP:CZ3	2.11	0.85
1:C:310:ILE:HG12	1:D:285:TYR:CD2	2.12	0.85
2:K:109:GLY:HA3	4:S:8:DT:O4'	1.77	0.84
3:R:6178:PHE:CD2	3:R:6180:PHE:HE2	1.96	0.84
2:A:90:SER:HB3	2:A:93:ALA:H	1.41	0.84
1:N:303:LEU:HD22	1:O:265:VAL:CG1	2.06	0.84
2:K:80:TYR:CZ	2:K:84:LEU:HD11	2.13	0.83
1:E:200:ASN:HD22	1:E:206:LYS:HG2	1.42	0.83
3:R:6196:LEU:HD13	3:R:6209:PHE:CE1	2.12	0.83
1:D:303:LEU:HD22	1:E:265:VAL:CG1	2.07	0.83
1:N:97:PHE:CE2	3:Q:5078:ASP:HA	2.13	0.83
1:O:57:THR:HG22	1:O:107:ASP:OD1	1.78	0.83
1:M:243:LYS:HG2	1:M:318:TRP:HE1	1.42	0.83
1:M:310:ILE:HG12	1:N:285:TYR:CD2	2.14	0.83
1:L:226:SER:O	1:L:230:ASN:HB2	1.77	0.83
1:L:277:THR:HG22	1:L:317:GLN:O	1.77	0.83
1:L:246:ASP:OD2	1:L:249:GLN:HG3	1.78	0.83
1:L:77:SER:HB3	1:L:111:ARG:NH1	1.94	0.83
1:D:88:LEU:HD22	1:D:104:ILE:HD13	1.59	0.83
1:L:81:ILE:HD11	1:L:120:HIS:CD2	2.14	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:97:PHE:CD2	3:Q:5079:GLY:N	2.47	0.83
3:G:5210:GLU:HA	3:G:5215:ASN:ND2	1.94	0.82
1:M:88:LEU:HD22	1:M:104:ILE:HD13	1.60	0.82
3:P:7109:PHE:CE2	3:P:7208:LYS:HB3	2.14	0.82
1:E:217:LYS:HE3	1:E:219:VAL:O	1.79	0.82
1:O:216:SER:OG	2:K:148:ASN:OD1	1.97	0.82
1:C:88:LEU:HD22	1:C:104:ILE:HD13	1.61	0.81
1:D:9:HIS:HD2	1:E:41:LYS:HB3	1.44	0.81
3:R:6027:GLN:HG2	3:R:6047:VAL:HA	1.63	0.81
1:E:246:ASP:OD2	1:E:249:GLN:HG3	1.80	0.81
3:G:5005:LYS:HE3	3:G:5069:ASP:OD1	1.79	0.81
1:E:61:LYS:HG2	1:E:71:MET:HE1	1.60	0.81
1:E:216:SER:OG	2:A:148:ASN:OD1	1.98	0.81
3:H:6030:MSE:HE3	3:H:6039:TYR:HE1	1.44	0.81
1:E:10:ILE:HD13	2:A:141:TYR:CE2	2.16	0.81
1:D:77:SER:HB3	1:D:111:ARG:NH1	1.96	0.80
4:I:29:DG:H2"	4:I:30:DC:OP2	1.80	0.80
1:C:246:ASP:OD2	1:C:249:GLN:HG3	1.81	0.80
3:P:7028:PHE:CZ	3:P:7030:MSE:HE2	2.16	0.80
3:G:5189:MSE:HB2	3:G:5216:TYR:CD2	2.15	0.80
2:K:109:GLY:HA2	4:S:8:DT:O2	1.82	0.80
1:B:226:SER:O	1:B:230:ASN:HB2	1.81	0.80
5:T:19:DT:H2"	5:T:20:DA:H5'	1.62	0.80
3:H:6030:MSE:HE3	3:H:6039:TYR:CE1	2.16	0.80
1:C:303:LEU:HD22	1:D:265:VAL:HG12	1.64	0.80
3:Q:5153:ASN:O	3:Q:5157:ASP:HB2	1.82	0.80
1:B:246:ASP:OD2	1:B:249:GLN:HG3	1.82	0.80
3:H:6030:MSE:HE2	3:H:6103:PRO:HB2	1.63	0.80
1:E:68:ASN:O	1:E:100:ARG:HD3	1.80	0.79
1:O:217:LYS:HE3	1:O:219:VAL:O	1.82	0.79
1:O:200:ASN:N	1:O:200:ASN:OD1	2.15	0.79
3:R:6082:LYS:HE3	3:R:6089:THR:HG21	1.63	0.79
2:K:50:LYS:HA	2:K:99:MET:HE3	1.65	0.79
5:J:3:DA:H1'	5:J:4:DG:H5'	1.64	0.79
2:A:80:TYR:CZ	2:A:84:LEU:HD11	2.18	0.79
3:H:6078:ASP:O	3:H:6080:ASN:N	2.15	0.79
3:R:6035:ASN:OD1	3:R:6037:THR:HG22	1.81	0.79
1:B:303:LEU:HD22	1:C:265:VAL:CG1	2.12	0.79
1:N:256:LYS:CE	1:O:159:GLN:HE22	1.93	0.79
1:E:10:ILE:HD13	2:A:141:TYR:CD2	2.18	0.79
2:A:145:LEU:HB3	2:A:151:LEU:HB2	1.63	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:6178:PHE:CD2	3:R:6180:PHE:CE2	2.71	0.78
1:D:77:SER:HB2	1:E:120:HIS:CD2	2.17	0.78
2:K:3:LEU:HG	3:P:7036:GLY:O	1.82	0.78
3:P:7226:HIS:HB2	3:P:7228:PHE:CD1	2.18	0.78
3:H:6032:ARG:HD3	3:H:6103:PRO:HA	1.64	0.78
1:B:118:GLN:OE1	1:B:145:ILE:HG23	1.84	0.78
3:H:6034:VAL:HG13	3:H:6101:VAL:HG21	1.65	0.78
5:T:3:DA:H2"	5:T:4:DG:H5'	1.64	0.78
2:K:145:LEU:HB3	2:K:151:LEU:HB2	1.65	0.78
3:H:6159:ALA:HB3	3:H:6161:THR:HG23	1.65	0.78
1:O:213:SER:HA	2:K:148:ASN:ND2	1.98	0.78
1:B:297:ILE:HG22	1:C:295:HIS:O	1.84	0.78
1:B:121:LEU:HD23	1:B:148:LEU:HD21	1.66	0.78
1:D:275:ARG:O	1:D:318:TRP:CD1	2.37	0.78
1:N:77:SER:HB3	1:N:111:ARG:NH1	1.97	0.78
3:F:7030:MSE:HE3	3:F:7103:PRO:HB2	1.64	0.78
3:F:7005:LYS:HG2	3:F:7006:ASP:N	1.99	0.78
3:F:7005:LYS:HG2	3:F:7006:ASP:H	1.47	0.78
1:M:299:ALA:HB2	1:N:295:HIS:HD2	1.47	0.78
1:D:95:ALA:HB2	3:G:5096:ASP:HB3	1.64	0.78
1:B:243:LYS:HG2	1:B:318:TRP:HE1	1.49	0.78
3:R:6115:VAL:HG13	3:R:6197:LEU:HD23	1.65	0.77
6:M:700:08T:C2'	6:M:700:08T:N3	2.43	0.77
1:B:243:LYS:HG2	1:B:318:TRP:NE1	1.99	0.77
3:G:5116:THR:HG23	3:G:5117:GLU:N	1.99	0.77
2:K:7:ASP:OD2	3:P:7032:ARG:NH2	2.17	0.77
1:D:97:PHE:CZ	3:G:5078:ASP:O	2.38	0.77
3:G:5157:ASP:HB2	3:G:5161:THR:HG23	1.67	0.77
1:N:246:ASP:OD2	1:N:249:GLN:HG3	1.85	0.77
3:P:7022:MSE:HE2	3:P:7024:LYS:HG3	1.67	0.77
1:E:277:THR:HG23	1:E:280:SER:HB2	1.65	0.77
1:D:310:ILE:HG12	1:E:285:TYR:HD2	1.49	0.77
3:R:6011:LEU:HB3	3:R:6061:LEU:HD11	1.65	0.77
2:A:38:ASN:O	4:I:9:DT:H73	1.85	0.77
1:M:77:SER:HB3	1:M:111:ARG:NH1	1.99	0.77
1:O:251:ARG:NE	2:K:71:GLN:HA	2.00	0.77
1:C:57:THR:OG1	6:C:700:08T:O1B	2.02	0.76
1:D:95:ALA:CB	3:G:5096:ASP:HB3	2.15	0.76
1:D:170:LYS:NZ	1:N:39:LYS:HG2	2.00	0.76
1:N:57:THR:OG1	6:N:700:08T:O1B	2.00	0.76
5:J:3:DA:H2"	5:J:4:DG:OP2	1.83	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:61:LYS:HG2	1:O:71:MET:HE1	1.67	0.76
1:D:256:LYS:HE3	1:E:159:GLN:NE2	2.00	0.76
5:J:9:DT:H2"	5:J:10:DA:H5'	1.66	0.76
2:K:142:LYS:O	2:K:146:THR:HG23	1.85	0.76
1:L:292:ASN:ND2	2:K:88:GLY:HA3	1.99	0.76
1:M:49:SER:HB3	1:M:56:LYS:HZ1	1.49	0.76
3:H:6180:PHE:CD2	3:H:6198:LEU:HD13	2.16	0.76
6:N:700:08T:H6	6:N:700:08T:N3	1.99	0.76
1:D:170:LYS:HZ1	1:N:39:LYS:CA	1.98	0.76
1:M:243:LYS:HG2	1:M:318:TRP:NE1	2.01	0.76
1:E:316:MET:CB	1:E:318:TRP:HZ3	1.98	0.75
1:O:68:ASN:O	1:O:100:ARG:HD3	1.86	0.75
1:D:108:GLU:HB3	1:E:122:ARG:NH2	2.01	0.75
3:H:6146:LYS:HA	3:H:6171:ASP:HA	1.68	0.75
3:F:7197:LEU:HD11	3:F:7210:GLU:OE2	1.86	0.75
1:B:248:LYS:HG2	1:C:273:TYR:HH	1.50	0.75
3:R:6129:VAL:HG11	3:R:6165:TYR:CD2	2.20	0.75
1:L:248:LYS:HG2	1:M:273:TYR:HH	1.50	0.75
2:A:4:PHE:CE2	3:F:7032:ARG:HD2	2.22	0.75
1:N:277:THR:HG23	1:N:280:SER:HB2	1.69	0.75
1:E:57:THR:HG22	1:E:107:ASP:OD1	1.86	0.75
1:M:303:LEU:HD22	1:N:265:VAL:CG1	2.15	0.75
2:K:150:LYS:C	2:K:152:PRO:HD3	2.07	0.75
1:E:108:GLU:H	1:E:137:THR:HB	1.51	0.75
1:C:243:LYS:HE2	1:C:318:TRP:HE1	1.50	0.75
3:H:6176:ASN:HB2	3:H:6227:ASP:OD1	1.87	0.75
1:L:121:LEU:HD23	1:L:148:LEU:HD21	1.69	0.75
1:C:9:HIS:HD2	1:D:41:LYS:CB	2.00	0.75
3:P:7118:ILE:HG12	3:P:7119:LYS:H	1.48	0.75
2:K:7:ASP:OD2	3:P:7032:ARG:CZ	2.35	0.75
2:A:50:LYS:HA	2:A:99:MET:HE3	1.67	0.75
1:O:246:ASP:OD2	1:O:249:GLN:HG3	1.86	0.75
3:P:7153:ASN:O	3:P:7157:ASP:HB3	1.86	0.75
3:G:5144:GLU:O	3:G:5146:LYS:HG3	1.85	0.74
3:G:5007:THR:HG23	3:G:5044:ILE:HG21	1.70	0.74
2:K:41:PHE:HD2	4:S:9:DT:H72	1.52	0.74
1:L:118:GLN:OE1	1:L:145:ILE:HG23	1.87	0.74
1:C:97:PHE:O	3:G:5204:GLN:HA	1.87	0.74
1:C:299:ALA:HB2	1:D:295:HIS:CD2	2.19	0.74
3:R:6013:ASN:ND2	3:R:6216:TYR:OH	2.20	0.74
2:K:155:LEU:CD2	2:K:183:LEU:HD21	2.18	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:200:ASN:N	1:E:200:ASN:OD1	2.18	0.74
1:C:72:MET:HE1	3:G:5035:ASN:CB	2.18	0.74
1:B:292:ASN:ND2	2:A:88:GLY:HA3	2.02	0.74
1:N:108:GLU:CB	1:O:122:ARG:HH21	1.93	0.74
3:H:6153:ASN:O	3:H:6157:ASP:HB2	1.87	0.74
3:H:6018:ASN:HB3	3:H:6031:THR:HG23	1.70	0.74
3:P:7109:PHE:CD2	3:P:7208:LYS:HD3	2.22	0.73
1:C:310:ILE:HG12	1:D:285:TYR:HD2	1.51	0.73
1:O:57:THR:HG23	8:O:700:ADP:O1B	1.88	0.73
1:C:9:HIS:CD2	1:D:41:LYS:CB	2.71	0.73
3:Q:5011:LEU:H	3:Q:5011:LEU:HD12	1.51	0.73
5:J:4:DG:H2"	5:J:5:DA:OP2	1.88	0.73
2:K:55:ILE:HG12	2:K:56:ALA:N	2.00	0.73
1:N:9:HIS:HD2	1:O:41:LYS:CB	2.01	0.73
1:B:277:THR:HG23	1:B:280:SER:HB2	1.71	0.73
2:A:55:ILE:HG12	2:A:56:ALA:N	2.04	0.73
1:B:57:THR:HG22	1:B:107:ASP:OD1	1.88	0.73
2:K:69:LEU:HD12	2:K:98:LEU:HD13	1.70	0.73
1:E:116:GLU:OE1	1:E:119:ARG:NH1	2.22	0.73
1:O:277:THR:HG23	1:O:280:SER:HB2	1.71	0.73
2:A:161:LEU:O	2:A:161:LEU:HG	1.89	0.73
3:R:6072:GLU:HB3	3:R:6084:ALA:HB3	1.71	0.73
1:D:48:HIS:NE2	1:D:141:ILE:HD11	2.03	0.72
1:E:176:LEU:HA	1:E:179:ILE:HD12	1.70	0.72
1:C:42:ILE:H	1:C:101:GLN:HE21	1.37	0.72
2:A:150:LYS:C	2:A:152:PRO:HD3	2.09	0.72
1:C:243:LYS:HG2	1:C:318:TRP:CZ2	2.25	0.72
3:G:5042:ALA:HB2	3:G:5214:ALA:HB2	1.71	0.72
3:R:6001:MSE:HG2	3:R:6073:ILE:O	1.89	0.72
1:C:277:THR:HG23	1:C:280:SER:HB2	1.71	0.72
3:R:6003:LEU:HD22	3:R:6007:THR:HG21	1.70	0.72
1:M:48:HIS:NE2	1:M:141:ILE:HD11	2.05	0.72
1:C:97:PHE:HB2	3:G:5205:GLY:O	1.90	0.72
3:R:6121:GLU:O	3:R:6124:GLN:HB3	1.90	0.72
3:P:7162:ARG:HG3	3:P:7162:ARG:HH11	1.53	0.72
3:P:7030:MSE:CE	3:P:7106:PRO:HB3	2.19	0.72
1:L:110:ASP:OD1	1:M:122:ARG:NH2	2.23	0.72
2:A:108:TYR:N	2:A:108:TYR:CD1	2.58	0.72
1:O:111:ARG:HB3	1:O:114:LEU:CD2	2.18	0.72
1:L:57:THR:CG2	1:L:137:THR:HG21	2.20	0.72
1:D:42:ILE:H	1:D:101:GLN:HE21	1.37	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:7014:PHE:HD2	3:F:7031:THR:HG22	1.54	0.72
1:N:49:SER:HB2	1:N:51:SER:O	1.90	0.72
1:L:57:THR:HG22	1:L:137:THR:HG21	1.71	0.71
1:E:118:GLN:OE1	1:E:145:ILE:HG23	1.90	0.71
1:O:200:ASN:HD22	1:O:206:LYS:HG2	1.54	0.71
1:B:316:MET:HB3	1:B:318:TRP:CZ3	2.25	0.71
3:R:6179:ASN:HB3	3:R:6225:THR:HG23	1.70	0.71
1:D:165:LYS:HE2	1:D:169:MET:HE2	1.70	0.71
1:E:251:ARG:HH21	2:A:71:GLN:HG2	1.53	0.71
3:G:5096:ASP:O	3:G:5098:SER:N	2.22	0.71
1:D:256:LYS:HE3	1:E:159:GLN:HE21	1.53	0.71
4:S:20:DG:N2	5:T:11:DC:O2	2.16	0.71
1:D:246:ASP:OD2	1:D:249:GLN:HG3	1.91	0.71
3:Q:5107:ILE:HG23	3:Q:5108:PRO:HD2	1.72	0.71
1:D:0:SER:HB2	1:D:2:ILE:H	1.56	0.71
3:P:7004:SER:O	3:P:7008:THR:HG23	1.90	0.71
1:N:49:SER:HB3	1:N:56:LYS:HZ1	1.54	0.71
1:D:49:SER:HB2	1:D:51:SER:O	1.90	0.71
1:D:49:SER:HB3	1:D:56:LYS:HZ2	1.54	0.71
1:E:243:LYS:HG2	1:E:318:TRP:HE1	1.54	0.71
1:O:15:TYR:O	1:O:175:ARG:NH2	2.23	0.71
1:N:175:ARG:HH11	1:N:175:ARG:HG3	1.56	0.71
3:P:7148:VAL:HG12	3:P:7168:THR:HG23	1.72	0.71
1:B:72:MET:HE2	3:G:5156:GLU:HA	1.71	0.71
1:C:277:THR:HG22	1:C:317:GLN:O	1.90	0.71
3:Q:5039:TYR:HD1	3:Q:5217:VAL:HG23	1.55	0.71
1:M:297:ILE:HD13	1:N:297:ILE:CD1	2.18	0.71
1:E:251:ARG:NE	2:A:71:GLN:HA	2.04	0.71
1:C:251:ARG:NH2	1:D:270:GLU:HG3	2.05	0.71
3:P:7030:MSE:HE1	3:P:7106:PRO:HB3	1.72	0.71
3:G:5042:ALA:HB2	3:G:5214:ALA:CB	2.20	0.71
1:E:111:ARG:HB3	1:E:114:LEU:CD2	2.17	0.71
1:N:276:VAL:HA	1:N:318:TRP:HB2	1.72	0.71
4:S:9:DT:H2'	4:S:9:DT:O2	1.89	0.71
2:A:71:GLN:OE1	2:A:111:TRP:HA	1.90	0.70
1:M:277:THR:HG22	1:M:317:GLN:O	1.90	0.70
2:A:109:GLY:HA3	4:I:8:DT:O4'	1.90	0.70
3:F:7227:ASP:O	3:F:7228:PHE:HB2	1.89	0.70
1:M:277:THR:HG23	1:M:280:SER:HB2	1.72	0.70
3:R:6138:ILE:HG12	3:R:6184:MSE:HE3	1.72	0.70
2:K:55:ILE:CG1	2:K:56:ALA:H	2.03	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:6135:ILE:HD13	3:R:6151:GLY:HA3	1.74	0.70
1:O:80:LYS:O	1:O:84:VAL:HG23	1.90	0.70
3:Q:5029:ILE:HG13	3:Q:5042:ALA:HB3	1.74	0.70
1:N:42:ILE:H	1:N:101:GLN:HE21	1.37	0.70
1:M:297:ILE:CD1	1:N:297:ILE:HD11	2.17	0.70
1:E:213:SER:HA	2:A:148:ASN:ND2	2.06	0.70
3:H:6018:ASN:HB3	3:H:6031:THR:CG2	2.21	0.70
5:T:3:DA:C2'	5:T:4:DG:H5'	2.22	0.70
3:H:6030:MSE:HE2	3:H:6103:PRO:CB	2.21	0.70
1:E:200:ASN:ND2	1:E:206:LYS:HG2	2.06	0.70
4:I:28:DT:H2"	4:I:29:DG:C8	2.27	0.70
3:R:6085:ASP:HB3	3:R:6088:SER:H	1.56	0.70
2:K:62:LYS:O	2:K:66:GLU:HB2	1.91	0.70
1:D:175:ARG:HG3	1:D:175:ARG:HH11	1.56	0.70
1:D:299:ALA:HB2	1:E:295:HIS:CD2	2.23	0.70
2:K:3:LEU:CD2	3:P:7219:ALA:HB2	2.22	0.70
4:I:14:DG:N2	5:J:17:DC:O2	2.23	0.70
3:F:7161:THR:HG23	3:F:7162:ARG:CG	2.21	0.70
1:M:119:ARG:HB3	1:M:122:ARG:HH12	1.57	0.70
3:P:7112:ALA:HB1	3:P:7114:ALA:O	1.92	0.70
6:N:700:08T:C2'	6:N:700:08T:N3	2.53	0.70
2:A:145:LEU:HB3	2:A:151:LEU:CB	2.21	0.69
1:E:243:LYS:HA	1:E:318:TRP:CZ2	2.26	0.69
1:D:119:ARG:HB3	1:D:122:ARG:HH12	1.57	0.69
3:G:5226:HIS:CD2	3:G:5228:PHE:HB2	2.27	0.69
3:Q:5129:VAL:CG1	3:Q:5133:LEU:HD12	2.22	0.69
1:O:26:PRO:HG3	1:O:160:PRO:HB3	1.74	0.69
3:G:5076:SER:O	3:G:5079:GLY:N	2.19	0.69
3:Q:5118:ILE:HG13	3:Q:5118:ILE:O	1.90	0.69
2:K:61:SER:HB3	2:K:64:MET:HB2	1.73	0.69
1:D:276:VAL:HA	1:D:318:TRP:HB2	1.73	0.69
1:D:170:LYS:HZ2	1:N:39:LYS:HG2	1.54	0.69
3:G:5021:ILE:CG2	3:G:5057:LEU:HD13	2.22	0.69
1:C:48:HIS:NE2	1:C:141:ILE:HD11	2.07	0.69
2:A:61:SER:HB3	2:A:64:MET:HB2	1.75	0.69
2:A:122:LEU:HD22	2:A:126:LEU:CD1	2.23	0.69
1:O:57:THR:OG1	8:O:700:ADP:O2A	2.09	0.69
1:L:285:TYR:HD2	2:K:97:TYR:HB2	1.58	0.69
6:B:700:08T:C2'	6:B:700:08T:N3	2.54	0.69
1:D:277:THR:HG23	1:D:280:SER:HB2	1.74	0.69
1:M:279:GLN:O	1:M:282:ILE:HG22	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:139:ASN:ND2	1:N:122:ARG:HE	1.90	0.69
1:C:175:ARG:HG3	1:C:175:ARG:HH11	1.56	0.69
3:G:5021:ILE:HG21	3:G:5057:LEU:HD13	1.75	0.69
3:G:5063:ILE:HD11	3:H:6133:LEU:HG	1.74	0.69
1:O:116:GLU:OE1	1:O:119:ARG:NH1	2.26	0.69
3:R:6120:ALA:HB2	3:R:6193:ASN:N	2.08	0.69
2:A:142:LYS:O	2:A:146:THR:HG23	1.92	0.69
1:B:17:PRO:HB3	1:B:22:GLU:HB3	1.74	0.69
2:A:122:LEU:HD22	2:A:126:LEU:HD12	1.75	0.68
1:B:16:ARG:NH2	6:B:700:08T:O2A	2.26	0.68
1:E:279:GLN:O	1:E:282:ILE:HG22	1.93	0.68
1:E:212:ASP:HB3	2:A:144:ILE:HG21	1.75	0.68
1:L:9:HIS:HD2	1:M:41:LYS:HB3	1.44	0.68
1:C:72:MET:HE1	3:G:5035:ASN:HB2	1.75	0.68
3:P:7120:ALA:HB2	3:P:7193:ASN:OD1	1.92	0.68
1:B:250:LEU:HD13	1:B:309:PHE:HB3	1.75	0.68
2:K:48:ASN:OD1	2:K:104:ARG:NH2	2.25	0.68
1:L:277:THR:HG23	1:L:280:SER:HB2	1.74	0.68
1:N:213:SER:HB3	1:O:153:ARG:CZ	2.24	0.68
3:F:7018:ASN:HD21	3:F:7034:VAL:HG23	1.58	0.68
1:C:77:SER:HB3	1:C:111:ARG:NH1	2.04	0.68
4:I:17:DC:H42	5:J:14:DG:H1	1.40	0.68
1:B:57:THR:CG2	1:B:137:THR:HG21	2.23	0.68
3:Q:5136:ASP:O	3:Q:5184:MSE:HB2	1.92	0.68
1:M:175:ARG:HG3	1:M:175:ARG:HH11	1.58	0.68
1:O:213:SER:C	2:K:148:ASN:HD21	1.97	0.68
6:L:700:08T:C2'	6:L:700:08T:N3	2.54	0.68
1:D:284:MET:HG3	1:D:285:TYR:N	2.07	0.68
1:D:167:GLU:OE1	1:N:38:SER:O	2.11	0.68
1:L:57:THR:HG22	1:L:107:ASP:OD1	1.94	0.68
5:T:19:DT:H2"	5:T:20:DA:C5'	2.23	0.68
3:P:7021:ILE:HG12	3:P:7022:MSE:N	2.09	0.68
3:R:6129:VAL:HG21	3:R:6165:TYR:CE2	2.29	0.68
1:B:57:THR:HG22	1:B:137:THR:HG21	1.76	0.68
3:Q:5136:ASP:OD1	3:Q:5154:LYS:HB3	1.92	0.68
2:K:138:ALA:O	2:K:141:TYR:HB2	1.93	0.68
1:O:118:GLN:OE1	1:O:145:ILE:HG23	1.94	0.68
4:I:25:DG:N2	5:J:6:DC:O2	2.19	0.68
2:A:156:LYS:O	2:A:159:LYS:HG2	1.95	0.68
3:Q:5123:LEU:O	3:Q:5123:LEU:HD12	1.93	0.68
3:G:5123:LEU:HD23	3:G:5191:PRO:HA	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:192:VAL:HG11	1:L:220:LEU:HB3	1.75	0.68
1:O:251:ARG:HH21	2:K:71:GLN:HG2	1.58	0.67
4:S:7:DT:H4'	4:S:8:DT:H5'	1.73	0.67
3:R:6027:GLN:NE2	3:R:6047:VAL:HB	2.08	0.67
3:H:6159:ALA:CB	3:H:6161:THR:HG23	2.24	0.67
1:E:12:GLU:OE1	1:E:205:ARG:HD2	1.94	0.67
2:A:62:LYS:O	2:A:66:GLU:HB2	1.92	0.67
1:D:294:TYR:CD2	1:E:293:GLN:NE2	2.62	0.67
1:C:49:SER:HB2	1:C:51:SER:O	1.93	0.67
1:E:57:THR:HG23	8:E:700:ADP:O1B	1.93	0.67
1:C:263:TRP:CZ2	1:C:267:LYS:HG3	2.29	0.67
1:D:170:LYS:HE3	1:N:39:LYS:HA	1.74	0.67
3:R:6129:VAL:HG21	3:R:6165:TYR:HE2	1.59	0.67
2:A:162:VAL:O	2:A:162:VAL:HG12	1.94	0.67
1:N:299:ALA:CB	1:O:295:HIS:HD2	2.03	0.67
3:G:5156:GLU:HG2	3:G:5162:ARG:NH2	2.09	0.67
1:E:253:LEU:HD23	2:A:114:LEU:HD11	1.76	0.67
1:M:42:ILE:H	1:M:101:GLN:HE21	1.41	0.67
1:D:57:THR:CG2	1:D:107:ASP:OD1	2.43	0.67
3:R:6023:LEU:HB3	3:R:6029:ILE:HG22	1.75	0.67
3:H:6003:LEU:HD22	3:H:6007:THR:HG21	1.77	0.67
1:D:25:LEU:HD21	1:D:157:PHE:HE2	1.60	0.67
1:M:29:ASP:HA	1:M:32:THR:HG22	1.75	0.67
3:P:7021:ILE:HG12	3:P:7022:MSE:H	1.60	0.67
2:K:150:LYS:HB3	2:K:152:PRO:HD3	1.75	0.67
1:M:42:ILE:H	1:M:101:GLN:NE2	1.92	0.67
1:M:49:SER:HB2	1:M:51:SER:O	1.94	0.67
5:J:4:DG:H2'	5:J:4:DG:OP2	1.95	0.67
2:A:150:LYS:HB3	2:A:152:PRO:HD3	1.76	0.67
2:K:120:GLU:OE2	2:K:142:LYS:NZ	2.28	0.67
5:J:9:DT:H2"	5:J:10:DA:OP2	1.93	0.67
1:C:243:LYS:HG2	1:C:318:TRP:CE2	2.30	0.67
2:K:126:LEU:HG	2:K:166:PHE:CE2	2.30	0.67
1:N:29:ASP:HA	1:N:32:THR:HG22	1.76	0.67
3:Q:5087:ARG:NH1	3:R:6122:ASP:OD2	2.28	0.67
3:Q:5120:ALA:HB2	3:Q:5192:GLY:C	2.14	0.67
1:E:26:PRO:HG3	1:E:160:PRO:HB3	1.76	0.67
1:D:297:ILE:HD13	1:E:297:ILE:CD1	2.25	0.66
3:P:7044:ILE:HG13	3:P:7045:SER:H	1.60	0.66
1:N:277:THR:HG22	1:N:317:GLN:O	1.94	0.66
2:K:7:ASP:O	2:K:8:ILE:C	2.33	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:72:MET:CE	3:R:6156:GLU:HA	2.25	0.66
3:P:7154:LYS:HA	3:P:7157:ASP:O	1.95	0.66
1:E:80:LYS:O	1:E:84:VAL:HG23	1.95	0.66
3:P:7050:PHE:CD2	3:P:7075:GLN:HB2	2.30	0.66
1:M:297:ILE:CG2	1:N:297:ILE:HG13	2.25	0.66
1:D:95:ALA:HB2	3:G:5096:ASP:CA	2.26	0.66
2:K:108:TYR:CD1	2:K:108:TYR:N	2.60	0.66
2:A:11:ASN:OD1	2:A:14:GLN:HG3	1.94	0.66
2:K:11:ASN:OD1	2:K:14:GLN:HG3	1.96	0.66
1:B:12:GLU:O	6:B:700:08T:O3'	2.12	0.66
2:A:120:GLU:OE2	2:A:142:LYS:NZ	2.29	0.66
2:A:124:ILE:HD13	2:A:139:ILE:CD1	2.25	0.66
3:F:7153:ASN:OD1	3:F:7155:VAL:HG13	1.94	0.66
2:K:161:LEU:HG	2:K:161:LEU:O	1.95	0.66
1:B:81:ILE:CD1	1:B:120:HIS:CD2	2.79	0.66
3:R:6011:LEU:CB	3:R:6061:LEU:HD21	2.24	0.66
1:L:285:TYR:CD2	2:K:97:TYR:HB2	2.30	0.66
3:F:7189:MSE:HE2	3:F:7209:PHE:CG	2.29	0.66
1:D:297:ILE:HG21	1:E:297:ILE:HG13	1.78	0.66
1:E:251:ARG:NH2	2:A:71:GLN:HG2	2.10	0.66
1:O:12:GLU:O	8:O:700:ADP:O3'	2.13	0.66
3:Q:5129:VAL:HG13	3:Q:5133:LEU:HD12	1.78	0.66
1:N:284:MET:HG3	1:N:285:TYR:N	2.08	0.66
4:I:27:DC:H2"	4:I:28:DT:OP2	1.94	0.66
3:H:6146:LYS:HG2	3:H:6171:ASP:HB3	1.77	0.66
3:H:6018:ASN:ND2	3:H:6020:GLY:O	2.28	0.66
3:Q:5039:TYR:HD1	3:Q:5217:VAL:CG2	2.08	0.66
1:E:250:LEU:HD13	1:E:309:PHE:HB3	1.77	0.66
2:K:145:LEU:HB3	2:K:151:LEU:CB	2.25	0.66
1:E:81:ILE:HG23	1:E:82:ASP:OD1	1.96	0.66
3:Q:5122:ASP:HB3	3:Q:5167:LEU:HD21	1.78	0.66
3:R:6135:ILE:HG23	3:R:6152:PHE:O	1.95	0.66
1:D:250:LEU:HD13	1:D:309:PHE:HB3	1.77	0.66
2:A:55:ILE:CG1	2:A:56:ALA:H	2.05	0.66
3:P:7028:PHE:CE2	3:P:7030:MSE:CE	2.79	0.66
3:R:6001:MSE:HE2	3:R:6003:LEU:HG	1.76	0.66
3:G:5034:VAL:HG23	3:G:5101:VAL:HG21	1.76	0.66
1:B:192:VAL:HG11	1:B:220:LEU:HB3	1.76	0.66
1:C:42:ILE:H	1:C:101:GLN:NE2	1.93	0.66
3:H:6189:MSE:HB2	3:H:6216:TYR:CE2	2.31	0.66
1:N:276:VAL:HA	1:N:318:TRP:CB	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:69:LEU:HD12	2:A:98:LEU:HD13	1.76	0.65
1:D:95:ALA:HB2	3:G:5096:ASP:CB	2.26	0.65
3:P:7134:GLN:HB3	3:P:7153:ASN:ND2	2.11	0.65
1:C:57:THR:CG2	1:C:107:ASP:OD1	2.43	0.65
1:B:284:MET:HG3	1:B:285:TYR:N	2.09	0.65
1:L:17:PRO:HB3	1:L:22:GLU:HB3	1.79	0.65
3:Q:5146:LYS:HA	3:Q:5171:ASP:HA	1.79	0.65
1:M:50:PRO:HA	1:M:139:ASN:O	1.95	0.65
1:D:50:PRO:HA	1:D:139:ASN:O	1.96	0.65
3:F:7054:ILE:HG22	3:F:7055:TYR:N	2.11	0.65
3:H:6210:GLU:HA	3:H:6215:ASN:ND2	2.12	0.65
3:G:5052:VAL:HG22	3:G:5053:ALA:N	2.11	0.65
1:C:279:GLN:O	1:C:282:ILE:HG22	1.96	0.65
2:A:143:SER:O	2:A:147:LYS:HB2	1.96	0.65
1:L:289:GLY:HA3	2:K:85:ILE:CG2	2.26	0.65
1:D:277:THR:CG2	1:D:317:GLN:O	2.44	0.65
1:D:9:HIS:HD2	1:E:41:LYS:CB	2.07	0.65
1:B:277:THR:HG22	1:B:317:GLN:O	1.96	0.65
3:R:6011:LEU:HB2	3:R:6061:LEU:HD21	1.78	0.65
1:L:284:MET:HG3	1:L:285:TYR:N	2.12	0.65
1:C:119:ARG:HB3	1:C:122:ARG:HH12	1.61	0.65
3:P:7123:LEU:O	3:P:7127:LEU:HG	1.96	0.65
3:G:5037:THR:HG21	3:G:5186:ASN:OD1	1.97	0.65
1:B:111:ARG:HB2	1:B:114:LEU:HD22	1.79	0.65
1:C:49:SER:HB3	1:C:56:LYS:HZ1	1.61	0.65
1:L:111:ARG:HB2	1:L:114:LEU:HD22	1.78	0.64
1:M:299:ALA:HB2	1:N:295:HIS:CD2	2.32	0.64
1:C:206:LYS:HD3	1:D:149:GLN:O	1.98	0.64
1:M:25:LEU:HD21	1:M:157:PHE:HE2	1.61	0.64
1:O:28:PHE:O	1:O:32:THR:HB	1.96	0.64
3:Q:5064:LEU:CD2	3:Q:5083:ILE:HD13	2.26	0.64
3:P:7109:PHE:CE2	3:P:7208:LYS:CB	2.79	0.64
3:F:7190:GLN:HG2	3:F:7216:TYR:OH	1.97	0.64
1:D:204:PHE:O	1:D:207:THR:HG22	1.97	0.64
1:M:297:ILE:HG21	1:N:297:ILE:HG13	1.79	0.64
2:A:155:LEU:CD2	2:A:183:LEU:HD21	2.26	0.64
3:P:7030:MSE:HE1	3:P:7106:PRO:CB	2.27	0.64
3:R:6085:ASP:OD1	3:R:6087:ARG:N	2.30	0.64
2:A:126:LEU:HG	2:A:166:PHE:CE2	2.32	0.64
1:B:232:ARG:CD	1:B:233:GLY:H	2.09	0.64
3:R:6023:LEU:CB	3:R:6029:ILE:HG22	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:279:GLN:O	1:O:282:ILE:HG22	1.98	0.64
1:D:191:LYS:HD3	1:M:186:ALA:HB2	1.79	0.64
1:N:48:HIS:NE2	1:N:141:ILE:HD11	2.11	0.64
1:E:147:PRO:O	1:E:151:ARG:HD2	1.98	0.64
1:E:303:LEU:HD11	2:A:76:MET:HE1	1.78	0.64
1:D:97:PHE:CD2	3:G:5079:GLY:HA3	2.32	0.64
1:N:42:ILE:H	1:N:101:GLN:NE2	1.95	0.64
3:G:5109:PHE:CE1	3:G:5208:LYS:HB2	2.32	0.64
3:F:7210:GLU:HG3	3:F:7215:ASN:ND2	2.13	0.64
1:D:191:LYS:HD3	1:M:186:ALA:CB	2.28	0.64
1:M:294:TYR:CD2	1:N:293:GLN:NE2	2.65	0.64
2:K:156:LYS:O	2:K:159:LYS:HG2	1.98	0.64
3:P:7041:GLU:O	3:P:7214:ALA:HB1	1.98	0.64
1:N:297:ILE:CG2	1:O:297:ILE:HG13	2.27	0.64
3:P:7122:ASP:HB3	3:P:7167:LEU:HD21	1.79	0.64
2:K:122:LEU:HD22	2:K:126:LEU:HD12	1.79	0.64
1:O:48:HIS:NE2	1:O:141:ILE:HD11	2.13	0.64
3:H:6130:SER:OG	3:H:6184:MSE:HE2	1.97	0.64
1:O:56:LYS:HA	1:O:157:PHE:HE2	1.63	0.64
1:L:9:HIS:HD2	1:M:41:LYS:HB2	1.63	0.64
1:N:50:PRO:HA	1:N:139:ASN:O	1.97	0.64
3:P:7226:HIS:HB2	3:P:7228:PHE:HD1	1.60	0.64
3:Q:5223:ASP:OD1	3:Q:5223:ASP:N	2.21	0.64
1:N:119:ARG:HB3	1:N:122:ARG:HH12	1.62	0.63
1:O:212:ASP:HB3	2:K:144:ILE:CG2	2.27	0.63
1:D:57:THR:CG2	1:D:137:THR:HG21	2.28	0.63
3:Q:5226:HIS:CE1	3:Q:5228:PHE:HB2	2.33	0.63
1:M:307:TYR:HE1	1:N:286:GLU:HA	1.63	0.63
1:C:25:LEU:HD21	1:C:157:PHE:HE2	1.63	0.63
3:G:5064:LEU:HD23	3:G:5064:LEU:O	1.98	0.63
3:P:7109:PHE:HE2	3:P:7208:LYS:HB3	1.59	0.63
1:M:97:PHE:O	3:Q:5204:GLN:CA	2.44	0.63
2:A:55:ILE:C	2:A:57:GLN:H	2.01	0.63
3:R:6063:ILE:HG21	3:R:6090:ILE:HG21	1.79	0.63
1:L:303:LEU:HD22	1:M:265:VAL:CG1	2.28	0.63
1:C:67:VAL:O	1:C:67:VAL:HG12	1.97	0.63
2:K:71:GLN:OE1	2:K:111:TRP:HA	1.97	0.63
1:N:242:LEU:HD12	1:N:250:LEU:HD21	1.81	0.63
1:L:292:ASN:ND2	2:K:88:GLY:O	2.32	0.63
1:L:242:LEU:HD12	1:L:250:LEU:HD21	1.81	0.63
2:K:43:ILE:O	2:K:47:ILE:HG13	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:260:ASP:OD2	1:C:50:PRO:CG	2.44	0.63
1:B:98:ASP:N	1:B:98:ASP:OD1	2.29	0.63
3:Q:5040:ALA:HB2	3:Q:5216:TYR:CD1	2.33	0.63
2:A:164:ASP:CA	2:A:167:LEU:HD12	2.17	0.63
3:G:5063:ILE:CD1	3:H:6133:LEU:HG	2.28	0.63
1:L:263:TRP:CZ2	1:L:267:LYS:HG3	2.34	0.63
3:P:7089:THR:HG22	3:P:7091:PHE:CE1	2.34	0.63
2:K:55:ILE:C	2:K:57:GLN:H	2.02	0.63
3:P:7028:PHE:CE2	3:P:7030:MSE:HE3	2.34	0.63
2:K:162:VAL:HG12	2:K:162:VAL:O	1.99	0.63
1:O:263:TRP:CZ2	1:O:267:LYS:HG3	2.34	0.63
1:N:297:ILE:HD13	1:O:297:ILE:CD1	2.23	0.62
1:L:276:VAL:HG23	1:L:318:TRP:HB3	1.81	0.62
3:R:6134:GLN:O	3:R:6153:ASN:ND2	2.32	0.62
5:T:4:DG:H2"	5:T:5:DA:OP2	2.00	0.62
3:H:6015:ALA:HB2	3:H:6057:LEU:HD23	1.81	0.62
1:D:307:TYR:CE1	1:E:286:GLU:HA	2.34	0.62
3:P:7034:VAL:HG13	3:P:7101:VAL:HG21	1.80	0.62
3:Q:5050:PHE:CD2	3:Q:5075:GLN:HB2	2.34	0.62
1:M:284:MET:HG3	1:M:285:TYR:N	2.11	0.62
1:B:293:GLN:NE2	1:E:297:ILE:CG2	2.62	0.62
1:N:57:THR:CG2	1:N:137:THR:HG21	2.29	0.62
4:S:26:DT:H3	5:T:5:DA:H61	1.45	0.62
3:R:6070:ASP:OD2	3:R:6086:ALA:HB2	1.98	0.62
2:K:122:LEU:HD22	2:K:126:LEU:CD1	2.29	0.62
1:O:165:LYS:HG2	1:O:169:MET:CE	2.29	0.62
1:O:276:VAL:HG23	1:O:318:TRP:HB3	1.81	0.62
1:N:263:TRP:CZ2	1:N:267:LYS:HG3	2.33	0.62
1:D:213:SER:HB3	1:E:153:ARG:CZ	2.29	0.62
3:F:7179:ASN:HB3	3:F:7225:THR:OG1	1.99	0.62
3:G:5157:ASP:HB2	3:G:5161:THR:CG2	2.29	0.62
1:D:42:ILE:H	1:D:101:GLN:NE2	1.97	0.62
3:F:7152:PHE:HB2	3:F:7160:LEU:HD22	1.81	0.62
3:P:7002:LYS:HE3	3:P:7070:ASP:O	2.00	0.62
3:H:6109:PHE:CD1	3:H:6110:PRO:HD2	2.35	0.62
1:D:29:ASP:HA	1:D:32:THR:HG22	1.79	0.62
1:B:49:SER:N	1:B:56:LYS:HD3	2.14	0.62
1:D:279:GLN:O	1:D:282:ILE:HG22	1.99	0.62
3:F:7026:GLY:H	3:F:7048:ILE:HB	1.65	0.62
1:L:98:ASP:N	1:L:98:ASP:OD1	2.32	0.62
1:C:29:ASP:HA	1:C:32:THR:HG22	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:307:TYR:HE1	1:E:286:GLU:HA	1.63	0.62
3:Q:5126:LEU:HD13	3:Q:5165:TYR:CE2	2.34	0.62
1:L:208:ILE:O	1:L:211:LEU:HB3	2.00	0.62
1:E:243:LYS:HG2	1:E:318:TRP:NE1	2.14	0.62
1:E:288:VAL:HG22	1:E:308:LEU:HD11	1.80	0.62
1:B:164:ASP:O	1:B:168:MET:HB2	1.98	0.62
3:Q:5078:ASP:C	3:Q:5080:ASN:H	2.02	0.62
1:E:56:LYS:HA	1:E:157:PHE:HE2	1.64	0.62
1:O:243:LYS:HG2	1:O:318:TRP:CZ2	2.35	0.62
3:Q:5055:TYR:HB2	3:Q:5095:ALA:HB2	1.81	0.62
1:M:54:THR:HG22	1:M:202:PRO:O	2.00	0.62
3:R:6126:LEU:HD12	3:R:6126:LEU:O	2.00	0.62
1:B:208:ILE:O	1:B:211:LEU:HB3	2.00	0.62
1:D:263:TRP:CZ2	1:D:267:LYS:HG3	2.35	0.62
1:L:81:ILE:CD1	1:L:116:GLU:HG3	2.30	0.62
4:I:24:DT:H2"	4:I:25:DG:H5"	1.82	0.62
3:F:7080:ASN:HA	3:F:7094:ALA:CB	2.25	0.61
1:B:44:HIS:CE1	1:B:133:SER:HA	2.34	0.61
1:N:20:ILE:HG22	1:N:66:ASP:OD2	2.01	0.61
3:H:6013:ASN:O	3:H:6016:THR:OG1	2.15	0.61
1:M:71:MET:CE	1:M:73:PHE:HD1	2.12	0.61
3:P:7109:PHE:CD2	3:P:7208:LYS:HB3	2.34	0.61
2:A:7:ASP:O	2:A:8:ILE:C	2.38	0.61
1:N:275:ARG:O	1:N:318:TRP:CD1	2.53	0.61
3:P:7028:PHE:HZ	3:P:7030:MSE:HE2	1.62	0.61
2:K:149:GLY:O	2:K:151:LEU:N	2.34	0.61
3:P:7022:MSE:HB3	3:P:7102:ALA:HB2	1.82	0.61
1:O:108:GLU:H	1:O:137:THR:HB	1.63	0.61
1:E:32:THR:O	1:E:36:ILE:HG13	1.99	0.61
1:N:310:ILE:HG12	1:O:285:TYR:HD2	1.64	0.61
1:N:67:VAL:HG12	1:N:67:VAL:O	2.00	0.61
1:B:116:GLU:OE1	1:B:119:ARG:NH1	2.33	0.61
1:C:20:ILE:HG22	1:C:66:ASP:OD2	2.00	0.61
2:K:34:GLU:HG2	2:K:34:GLU:O	2.00	0.61
3:H:6002:LYS:O	3:H:6003:LEU:HD23	1.99	0.61
1:N:279:GLN:O	1:N:282:ILE:HG22	2.01	0.61
2:A:60:TYR:CE2	2:A:95:PHE:HB2	2.35	0.61
1:L:293:GLN:NE2	1:O:297:ILE:HG22	2.15	0.61
2:K:151:LEU:HG	2:K:151:LEU:O	1.99	0.61
3:Q:5053:ALA:HB3	3:Q:5095:ALA:O	2.00	0.61
2:K:124:ILE:HD13	2:K:139:ILE:CD1	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:57:THR:CG2	1:C:137:THR:HG21	2.31	0.61
2:K:60:TYR:CE2	2:K:95:PHE:HB2	2.35	0.61
1:D:33:PHE:O	1:D:37:THR:HG23	2.00	0.61
1:D:297:ILE:CG2	1:E:297:ILE:HG13	2.31	0.61
3:G:5135:ILE:HD13	3:G:5151:GLY:CA	2.23	0.61
2:K:76:MET:N	2:K:77:PRO:HD2	2.16	0.61
3:G:5096:ASP:C	3:G:5098:SER:H	2.03	0.61
3:Q:5200:ALA:HB1	3:Q:5226:HIS:NE2	2.15	0.61
1:C:33:PHE:O	1:C:37:THR:HG23	2.00	0.61
1:B:89:THR:HG22	3:F:7055:TYR:OH	2.01	0.61
3:R:6163:VAL:O	3:R:6163:VAL:HG22	2.01	0.61
3:H:6163:VAL:O	3:H:6163:VAL:HG13	2.00	0.61
1:E:28:PHE:O	1:E:32:THR:HB	2.00	0.61
1:L:44:HIS:CE1	1:L:133:SER:HA	2.35	0.61
1:N:297:ILE:HG21	1:O:297:ILE:HG13	1.81	0.61
1:O:159:GLN:O	1:O:159:GLN:HG3	2.01	0.61
1:M:47:LEU:HD22	1:M:157:PHE:HE1	1.65	0.61
2:A:20:LYS:HD2	3:F:7019:SER:HB2	1.82	0.61
1:N:25:LEU:HD21	1:N:157:PHE:HE2	1.66	0.61
1:L:293:GLN:CD	2:K:84:LEU:O	2.39	0.60
2:K:164:ASP:CA	2:K:167:LEU:HD12	2.14	0.60
3:P:7007:THR:HG23	3:P:7044:ILE:HG21	1.82	0.60
1:D:97:PHE:CE2	3:G:5078:ASP:C	2.75	0.60
3:R:6129:VAL:HG11	3:R:6165:TYR:HD2	1.65	0.60
1:O:242:LEU:HD12	1:O:250:LEU:HD21	1.83	0.60
1:L:293:GLN:NE2	1:O:297:ILE:CG2	2.64	0.60
3:Q:5076:SER:HB3	3:Q:5078:ASP:O	2.00	0.60
1:N:57:THR:CG2	1:N:107:ASP:OD1	2.45	0.60
1:O:61:LYS:HA	1:O:71:MET:HE3	1.84	0.60
1:B:242:LEU:HD12	1:B:250:LEU:HD21	1.82	0.60
1:M:263:TRP:CZ2	1:M:267:LYS:HG3	2.36	0.60
1:C:9:HIS:HD2	1:D:41:LYS:HB2	1.65	0.60
1:B:72:MET:CE	3:G:5156:GLU:HA	2.31	0.60
1:L:292:ASN:HD21	2:K:88:GLY:HA3	1.66	0.60
1:O:318:TRP:O	1:O:319:LYS:HG3	2.00	0.60
3:P:7210:GLU:HG2	3:P:7215:ASN:OD1	2.01	0.60
3:P:7125:GLN:O	3:P:7129:VAL:HG23	2.02	0.60
1:O:3:THR:HG21	1:O:18:SER:HB2	1.82	0.60
4:S:24:DT:H3	5:T:7:DA:H61	1.48	0.60
1:L:71:MET:HE3	1:L:105:VAL:HG21	1.82	0.60
1:O:304:HIS:HB2	2:K:83:ASN:ND2	2.17	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:143:SER:O	2:K:147:LYS:HB2	2.02	0.60
1:L:49:SER:N	1:L:56:LYS:HD3	2.17	0.60
1:N:256:LYS:CD	1:O:159:GLN:HE22	2.15	0.60
1:C:310:ILE:HG12	1:D:285:TYR:CE2	2.35	0.60
3:P:7022:MSE:HB3	3:P:7102:ALA:CB	2.31	0.60
5:J:3:DA:H1'	5:J:4:DG:C5'	2.32	0.60
2:A:14:GLN:HB3	2:A:18:TYR:CE2	2.37	0.60
4:S:27:DC:H2"	4:S:28:DT:H71	1.84	0.60
2:K:85:ILE:O	2:K:89:LEU:HD12	2.02	0.60
3:R:6163:VAL:O	3:R:6163:VAL:CG2	2.49	0.60
1:N:165:LYS:HE2	1:N:169:MET:HE2	1.84	0.60
1:M:220:LEU:HA	1:M:224:ILE:HD12	1.84	0.60
1:L:75:ASN:HB3	1:L:78:ASP:HB2	1.84	0.60
2:A:76:MET:N	2:A:77:PRO:HD2	2.17	0.60
1:D:242:LEU:HD12	1:D:250:LEU:HD21	1.83	0.60
2:A:173:ASN:O	2:A:176:GLU:HB3	2.02	0.60
1:E:165:LYS:HG2	1:E:169:MET:CE	2.32	0.60
1:N:242:LEU:HB3	1:N:318:TRP:HH2	1.65	0.60
1:N:169:MET:O	1:N:173:ILE:HG13	2.02	0.60
1:C:189:ASP:O	1:C:192:VAL:HG12	2.01	0.60
1:B:81:ILE:CD1	1:B:116:GLU:HG3	2.32	0.59
1:C:49:SER:HB3	1:C:56:LYS:HZ2	1.65	0.59
2:A:127:LEU:HD13	2:A:141:TYR:HB3	1.84	0.59
3:P:7130:SER:OG	3:P:7135:ILE:HB	2.02	0.59
3:F:7226:HIS:NE2	3:F:7227:ASP:O	2.34	0.59
2:A:64:MET:SD	4:I:10:DT:O2	2.60	0.59
1:M:250:LEU:HD13	1:M:309:PHE:HB3	1.84	0.59
1:M:33:PHE:O	1:M:37:THR:HG23	2.01	0.59
1:D:297:ILE:CD1	1:E:297:ILE:HD11	2.28	0.59
1:M:57:THR:CG2	1:M:137:THR:HG21	2.32	0.59
2:A:48:ASN:OD1	2:A:104:ARG:NH2	2.35	0.59
3:P:7226:HIS:HB2	3:P:7228:PHE:CE1	2.37	0.59
1:N:15:TYR:O	1:N:175:ARG:NH2	2.34	0.59
3:G:5056:ASP:O	3:G:5056:ASP:OD1	2.19	0.59
1:M:121:LEU:O	1:M:125:MET:HG3	2.03	0.59
1:E:61:LYS:HA	1:E:71:MET:HE3	1.84	0.59
3:H:6078:ASP:C	3:H:6080:ASN:H	2.03	0.59
2:A:151:LEU:HG	2:A:151:LEU:O	2.00	0.59
3:Q:5150:ASN:OD1	3:Q:5166:SER:OG	2.19	0.59
1:E:42:ILE:HG22	1:E:43:PRO:O	2.03	0.59
1:N:297:ILE:CD1	1:O:297:ILE:HD11	2.25	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:7010:LEU:O	3:P:7014:PHE:HD1	1.84	0.59
3:R:6209:PHE:N	3:R:6216:TYR:O	2.20	0.59
1:E:10:ILE:CD1	2:A:141:TYR:CE2	2.85	0.59
1:D:256:LYS:CE	1:E:159:GLN:NE2	2.65	0.59
1:M:165:LYS:HE2	1:M:169:MET:HE1	1.84	0.59
3:R:6017:ILE:HG12	3:R:6188:LYS:HB2	1.85	0.59
1:B:276:VAL:HG23	1:B:318:TRP:HB3	1.85	0.59
1:M:303:LEU:HD22	1:N:265:VAL:HG12	1.83	0.59
1:E:242:LEU:HD12	1:E:250:LEU:HD21	1.82	0.59
1:E:17:PRO:HB3	1:E:22:GLU:HB3	1.85	0.59
1:N:192:VAL:HG11	1:N:220:LEU:HB3	1.83	0.59
1:N:243:LYS:HG2	1:N:318:TRP:CZ2	2.37	0.59
3:P:7002:LYS:O	3:P:7003:LEU:HD23	2.03	0.59
1:M:242:LEU:HD12	1:M:250:LEU:HD21	1.85	0.59
1:M:139:ASN:HD22	1:N:122:ARG:HE	1.49	0.59
1:B:81:ILE:O	1:B:85:ARG:HG3	2.03	0.59
3:G:5156:GLU:CG	3:G:5162:ARG:HH21	2.13	0.59
2:A:138:ALA:O	2:A:141:TYR:HB2	2.02	0.59
3:F:7007:THR:HG23	3:F:7044:ILE:HG12	1.85	0.59
1:N:47:LEU:HD22	1:N:157:PHE:HE1	1.68	0.59
1:L:164:ASP:O	1:L:168:MET:HB2	2.03	0.59
3:G:5128:ARG:HB3	3:F:7066:LEU:HD13	1.84	0.59
1:C:294:TYR:CD2	1:D:293:GLN:NE2	2.71	0.59
3:F:7018:ASN:ND2	3:F:7034:VAL:HG23	2.18	0.59
1:M:307:TYR:CE1	1:N:286:GLU:HA	2.38	0.59
1:E:169:MET:O	1:E:173:ILE:HG13	2.03	0.59
3:G:5092:TRP:CD1	3:G:5093:PRO:HD2	2.38	0.59
3:P:7085:ASP:HB3	3:P:7088:SER:H	1.67	0.59
3:Q:5210:GLU:HG3	3:Q:5215:ASN:HD21	1.68	0.59
2:K:149:GLY:C	2:K:151:LEU:H	2.05	0.59
1:M:294:TYR:HB2	1:N:293:GLN:HE21	1.68	0.59
2:K:173:ASN:O	2:K:176:GLU:HB3	2.02	0.59
3:F:7085:ASP:CG	3:F:7086:ALA:H	2.07	0.59
1:B:263:TRP:CZ2	1:B:267:LYS:HG3	2.38	0.59
1:E:252:ALA:HB2	2:A:112:ALA:HB1	1.83	0.59
1:L:81:ILE:CD1	1:L:120:HIS:CD2	2.85	0.59
3:R:6138:ILE:HD12	3:R:6149:ILE:CG2	2.32	0.59
1:E:12:GLU:OE1	1:E:205:ARG:CD	2.51	0.59
1:B:110:ASP:OD1	1:C:122:ARG:NH2	2.35	0.59
1:O:173:ILE:HG23	1:O:193:VAL:CG1	2.33	0.59
1:M:192:VAL:HG11	1:M:220:LEU:HB3	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:6210:GLU:HA	3:R:6215:ASN:ND2	2.18	0.59
3:Q:5116:THR:HB	3:Q:5147:ILE:HD12	1.83	0.59
3:Q:5021:ILE:HG12	3:Q:5022:MSE:N	2.18	0.59
2:A:109:GLY:HA2	4:I:8:DT:O2	2.03	0.58
1:L:201:PHE:O	1:L:202:PRO:C	2.36	0.58
1:C:303:LEU:HD22	1:D:265:VAL:HG11	1.82	0.58
3:G:5023:LEU:HD11	3:G:5052:VAL:HG12	1.85	0.58
3:H:6073:ILE:HA	3:H:6082:LYS:O	2.02	0.58
3:P:7109:PHE:CD2	3:P:7208:LYS:CB	2.86	0.58
1:B:48:HIS:CE1	1:B:141:ILE:CD1	2.83	0.58
3:G:5034:VAL:CG2	3:G:5101:VAL:HG21	2.33	0.58
3:Q:5226:HIS:ND1	3:Q:5228:PHE:HB2	2.18	0.58
1:C:47:LEU:HD22	1:C:157:PHE:HE1	1.69	0.58
3:P:7007:THR:CG2	3:P:7044:ILE:HG21	2.33	0.58
1:O:200:ASN:ND2	1:O:206:LYS:HG2	2.17	0.58
3:R:6038:THR:HA	3:R:6218:VAL:HG12	1.85	0.58
2:K:152:PRO:CD	2:K:153:LEU:H	2.16	0.58
1:M:119:ARG:HB3	1:M:122:ARG:NH1	2.18	0.58
1:C:71:MET:CE	1:C:73:PHE:HD1	2.15	0.58
1:N:33:PHE:O	1:N:37:THR:HG23	2.03	0.58
1:E:303:LEU:CD1	2:A:70:SER:HB2	2.34	0.58
1:L:232:ARG:HH11	1:L:233:GLY:H	1.51	0.58
1:E:48:HIS:HB2	1:E:138:ALA:O	2.04	0.58
2:K:38:ASN:O	4:S:9:DT:H73	2.02	0.58
3:H:6194:TYR:HH	3:H:6216:TYR:HE2	1.49	0.58
3:Q:5126:LEU:HD13	3:Q:5165:TYR:HE2	1.69	0.58
4:I:29:DG:H2'	4:I:29:DG:O5'	2.03	0.58
1:O:284:MET:HG3	1:O:285:TYR:N	2.16	0.58
1:E:263:TRP:CZ2	1:E:267:LYS:HG3	2.37	0.58
2:A:85:ILE:O	2:A:89:LEU:HD12	2.04	0.58
2:A:149:GLY:C	2:A:151:LEU:H	2.07	0.58
1:E:284:MET:HG3	1:E:285:TYR:N	2.17	0.58
1:L:71:MET:CE	1:L:105:VAL:HG21	2.34	0.58
1:C:242:LEU:HD12	1:C:250:LEU:HD21	1.85	0.58
3:G:5165:TYR:HD1	3:F:7090:ILE:HG13	1.69	0.58
1:O:251:ARG:NH2	2:K:71:GLN:HG2	2.19	0.58
2:K:102:VAL:CG2	2:K:104:ARG:HH21	2.17	0.58
1:D:49:SER:HB3	1:D:56:LYS:HZ1	1.68	0.58
3:P:7135:ILE:HD11	3:P:7165:TYR:HB3	1.86	0.58
1:M:3:THR:OG1	1:M:22:GLU:OE1	2.21	0.58
2:A:34:GLU:HG2	2:A:34:GLU:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:116:GLU:OE2	1:N:119:ARG:NH1	2.37	0.58
1:E:303:LEU:HD11	2:A:76:MET:CE	2.34	0.58
1:C:139:ASN:ND2	1:D:122:ARG:HE	2.02	0.58
1:D:47:LEU:HD22	1:D:157:PHE:HE1	1.67	0.58
1:B:232:ARG:CG	1:B:233:GLY:H	2.17	0.58
3:Q:5189:MSE:HB2	3:Q:5216:TYR:CE2	2.39	0.58
1:O:165:LYS:HG2	1:O:169:MET:HE3	1.85	0.58
1:N:189:ASP:O	1:N:192:VAL:HG12	2.04	0.58
3:G:5180:PHE:CD2	3:G:5198:LEU:HD22	2.39	0.58
1:C:284:MET:HG3	1:C:285:TYR:N	2.17	0.58
2:K:80:TYR:CE1	2:K:84:LEU:HD11	2.38	0.57
1:D:294:TYR:HB2	1:E:293:GLN:HE21	1.69	0.57
3:F:7054:ILE:CG2	3:F:7055:TYR:N	2.66	0.57
1:B:251:ARG:NH1	1:C:285:TYR:OH	2.37	0.57
1:M:226:SER:O	1:M:230:ASN:HA	2.04	0.57
1:M:20:ILE:HG22	1:M:66:ASP:OD2	2.03	0.57
1:D:243:LYS:HG2	1:D:318:TRP:CZ2	2.38	0.57
1:D:276:VAL:HA	1:D:318:TRP:CB	2.34	0.57
1:M:57:THR:CG2	1:M:107:ASP:OD1	2.49	0.57
1:N:238:VAL:HG22	1:N:253:LEU:HD13	1.86	0.57
1:D:119:ARG:HB3	1:D:122:ARG:NH1	2.18	0.57
1:E:243:LYS:HA	1:E:318:TRP:HZ2	1.68	0.57
6:N:700:08T:F1	6:N:700:08T:O1B	2.11	0.57
1:C:50:PRO:HA	1:C:139:ASN:O	2.05	0.57
3:Q:5107:ILE:CG2	3:Q:5108:PRO:HD2	2.34	0.57
1:O:243:LYS:HA	1:O:318:TRP:CZ2	2.40	0.57
1:D:233:GLY:HA2	1:D:267:LYS:HE2	1.86	0.57
1:O:17:PRO:HB3	1:O:22:GLU:HB3	1.85	0.57
1:E:48:HIS:NE2	1:E:141:ILE:HD11	2.19	0.57
1:E:159:GLN:HG3	1:E:159:GLN:O	2.03	0.57
1:B:57:THR:CG2	1:B:107:ASP:OD1	2.52	0.57
1:E:141:ILE:O	1:E:144:ILE:N	2.37	0.57
3:R:6024:LYS:HB3	3:R:6051:ASP:OD1	2.04	0.57
3:G:5145:GLY:O	3:G:5172:TYR:N	2.28	0.57
3:P:7044:ILE:HG13	3:P:7045:SER:N	2.18	0.57
3:P:7023:LEU:O	3:P:7023:LEU:HD12	2.04	0.57
3:Q:5149:ILE:O	3:Q:5166:SER:HA	2.04	0.57
1:N:220:LEU:HA	1:N:224:ILE:HD12	1.86	0.57
1:D:71:MET:CE	1:D:73:PHE:HD1	2.17	0.57
3:Q:5078:ASP:O	3:Q:5080:ASN:N	2.38	0.57
1:O:15:TYR:CZ	1:O:179:ILE:HG23	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:108:TYR:HB3	4:S:7:DT:H72	1.86	0.57
3:Q:5010:LEU:O	3:Q:5013:ASN:HB3	2.05	0.57
1:O:83:PHE:O	1:O:87:PRO:HD2	2.04	0.57
1:C:48:HIS:NE2	1:C:156:THR:HB	2.20	0.57
1:D:57:THR:HG23	1:D:137:THR:HG21	1.86	0.57
1:E:11:LEU:HG	1:E:212:ASP:CG	2.25	0.57
1:L:250:LEU:HD13	1:L:309:PHE:HB3	1.87	0.57
3:F:7146:LYS:HA	3:F:7171:ASP:HA	1.87	0.57
1:C:297:ILE:CG2	1:D:297:ILE:HG13	2.34	0.57
6:C:700:08T:N3	6:C:700:08T:H6	2.15	0.57
1:B:72:MET:HE1	1:B:91:PHE:HB2	1.86	0.57
3:F:7056:ASP:HB3	3:F:7092:TRP:CZ2	2.25	0.57
1:D:170:LYS:NZ	1:N:39:LYS:CG	2.68	0.57
2:A:152:PRO:CD	2:A:153:LEU:H	2.17	0.57
1:N:165:LYS:HG2	1:N:169:MET:CE	2.34	0.57
1:O:83:PHE:CE1	1:O:87:PRO:HG2	2.40	0.57
3:R:6049:ASP:OD1	3:R:6050:PHE:HD1	1.88	0.57
2:A:43:ILE:O	2:A:47:ILE:HG13	2.05	0.56
1:E:251:ARG:HH11	1:E:251:ARG:CG	2.18	0.56
1:C:204:PHE:O	1:C:207:THR:HG22	2.05	0.56
3:P:7118:ILE:HG22	3:P:7194:TYR:O	2.05	0.56
3:R:6063:ILE:CG2	3:R:6090:ILE:HG21	2.35	0.56
1:C:119:ARG:HB3	1:C:122:ARG:NH1	2.20	0.56
3:R:6210:GLU:HG3	3:R:6215:ASN:HD21	1.70	0.56
1:O:42:ILE:HG22	1:O:43:PRO:O	2.04	0.56
2:K:4:PHE:CZ	3:P:7032:ARG:HD2	2.40	0.56
2:K:41:PHE:HA	2:K:44:ILE:HD12	1.86	0.56
2:A:149:GLY:O	2:A:151:LEU:N	2.38	0.56
3:G:5157:ASP:CB	3:G:5161:THR:HG23	2.35	0.56
3:P:7022:MSE:HE3	3:P:7023:LEU:O	2.04	0.56
1:B:232:ARG:CG	1:B:233:GLY:N	2.69	0.56
3:P:7121:GLU:O	3:P:7125:GLN:N	2.30	0.56
1:C:46:ILE:HB	1:C:154:VAL:HG22	1.87	0.56
1:O:251:ARG:HH11	1:O:251:ARG:CG	2.17	0.56
1:L:9:HIS:CD2	1:M:41:LYS:CB	2.69	0.56
3:G:5023:LEU:HD11	3:G:5052:VAL:CG1	2.35	0.56
1:O:57:THR:CG2	1:O:107:ASP:OD1	2.51	0.56
1:C:97:PHE:O	3:G:5204:GLN:CA	2.53	0.56
3:P:7167:LEU:HD12	3:P:7168:THR:N	2.20	0.56
1:C:238:VAL:HG22	1:C:253:LEU:HD13	1.86	0.56
1:L:72:MET:HE3	1:L:91:PHE:CG	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:5:ASN:O	1:B:7:LYS:N	2.38	0.56
3:Q:5034:VAL:HG22	3:Q:5101:VAL:HG21	1.86	0.56
1:E:33:PHE:CZ	1:E:59:VAL:HG11	2.41	0.56
1:C:121:LEU:O	1:C:125:MET:HG3	2.05	0.56
3:Q:5181:ILE:HB	3:Q:5221:GLU:HB2	1.86	0.56
1:D:67:VAL:HG12	1:D:67:VAL:O	2.03	0.56
1:B:77:SER:CB	1:B:111:ARG:HH11	2.05	0.56
1:N:243:LYS:HG2	1:N:318:TRP:CE2	2.41	0.56
1:M:98:ASP:HA	3:Q:5204:GLN:HG2	1.87	0.56
1:D:232:ARG:C	1:D:234:ALA:H	2.09	0.56
1:E:10:ILE:CD1	2:A:141:TYR:HE2	2.18	0.56
5:J:8:DC:H2"	5:J:9:DT:OP2	2.06	0.56
1:E:57:THR:OG1	8:E:700:ADP:O2A	2.23	0.56
1:E:15:TYR:O	1:E:175:ARG:NH2	2.39	0.56
1:C:230:ASN:C	1:C:230:ASN:OD1	2.43	0.56
1:C:110:ASP:OD1	1:D:122:ARG:NH2	2.39	0.56
1:M:243:LYS:HG2	1:M:318:TRP:CE2	2.41	0.56
1:O:95:ALA:CB	3:R:6220:LEU:O	2.54	0.56
3:F:7226:HIS:CG	3:F:7227:ASP:N	2.74	0.56
1:B:49:SER:HB2	1:B:51:SER:O	2.05	0.56
3:P:7123:LEU:HD23	3:P:7191:PRO:HA	1.88	0.56
3:P:7042:ALA:HB2	3:P:7214:ALA:CB	2.35	0.56
2:A:33:LYS:O	2:A:35:LYS:HG3	2.06	0.56
4:I:21:DT:H2"	4:I:22:DA:C8	2.41	0.56
1:N:16:ARG:HB2	6:N:700:08T:O3'	2.04	0.56
3:Q:5064:LEU:HD23	3:Q:5083:ILE:HD13	1.87	0.56
1:E:273:TYR:CD1	1:E:281:ILE:HD13	2.41	0.56
5:J:1:DG:H2"	5:J:2:DC:O4'	2.06	0.56
2:K:155:LEU:HD22	2:K:183:LEU:CD2	2.27	0.56
1:O:147:PRO:O	1:O:151:ARG:HD2	2.05	0.56
3:H:6030:MSE:HE2	3:H:6103:PRO:CG	2.36	0.56
3:G:5209:PHE:N	3:G:5216:TYR:O	2.31	0.56
4:S:27:DC:H2"	4:S:28:DT:OP2	2.06	0.56
1:C:226:SER:O	1:C:230:ASN:HA	2.06	0.56
1:O:251:ARG:HG3	1:O:251:ARG:HH11	1.70	0.56
1:O:165:LYS:O	1:O:169:MET:HG3	2.06	0.56
1:O:250:LEU:HD13	1:O:309:PHE:HB3	1.88	0.56
1:L:72:MET:HE3	1:L:91:PHE:CD1	2.41	0.56
1:E:83:PHE:CE1	1:E:87:PRO:HG2	2.40	0.56
1:M:68:ASN:O	1:M:100:ARG:HD3	2.06	0.56
1:B:80:LYS:NZ	4:I:19:DC:P	2.79	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:114:LEU:N	1:E:114:LEU:CD1	2.69	0.55
1:N:119:ARG:HB3	1:N:122:ARG:NH1	2.22	0.55
1:B:48:HIS:CG	1:B:141:ILE:HG12	2.40	0.55
1:M:243:LYS:HG2	1:M:318:TRP:CZ2	2.41	0.55
3:H:6152:PHE:HD2	3:H:6162:ARG:O	1.89	0.55
3:P:7167:LEU:HD12	3:P:7168:THR:H	1.71	0.55
1:M:189:ASP:O	1:M:192:VAL:HG12	2.07	0.55
1:E:83:PHE:O	1:E:87:PRO:HD2	2.05	0.55
3:F:7149:ILE:O	3:F:7166:SER:HA	2.06	0.55
1:N:71:MET:CE	1:N:73:PHE:HD1	2.19	0.55
1:C:205:ARG:NH2	6:C:700:08T:O2A	2.39	0.55
1:L:316:MET:HB3	1:L:318:TRP:CZ3	2.41	0.55
1:E:173:ILE:HG23	1:E:193:VAL:CG1	2.37	0.55
1:L:232:ARG:HG3	1:L:233:GLY:N	2.22	0.55
1:L:279:GLN:O	1:L:282:ILE:HG22	2.06	0.55
3:G:5032:ARG:HB3	3:G:5103:PRO:HG3	1.86	0.55
3:Q:5128:ARG:CG	3:P:7066:LEU:HD13	2.17	0.55
1:O:114:LEU:N	1:O:114:LEU:CD1	2.69	0.55
1:D:276:VAL:CG2	1:D:318:TRP:HB3	2.23	0.55
2:A:4:PHE:CZ	3:F:7032:ARG:HD2	2.42	0.55
2:A:161:LEU:HD12	2:A:163:THR:HG23	1.88	0.55
2:K:85:ILE:HG22	2:K:89:LEU:HD11	1.89	0.55
2:K:69:LEU:CD1	2:K:98:LEU:HD13	2.35	0.55
3:P:7136:ASP:OD2	3:P:7155:VAL:HG23	2.06	0.55
3:Q:5223:ASP:O	3:Q:5225:THR:HG23	2.05	0.55
3:R:6016:THR:OG1	3:R:6188:LYS:HB3	2.07	0.55
3:Q:5180:PHE:HE2	3:Q:5198:LEU:HB3	1.71	0.55
2:K:3:LEU:HD21	3:P:7219:ALA:CB	2.31	0.55
2:A:183:LEU:O	2:A:187:TRP:CD1	2.59	0.55
1:E:251:ARG:HH11	1:E:251:ARG:HG3	1.70	0.55
3:R:6197:LEU:HD12	3:R:6208:LYS:HG2	1.89	0.55
3:R:6125:GLN:O	3:R:6129:VAL:HG23	2.07	0.55
2:A:41:PHE:HA	2:A:44:ILE:HD12	1.87	0.55
1:M:67:VAL:HG12	1:M:67:VAL:O	2.06	0.55
1:D:77:SER:HA	1:D:114:LEU:HD11	1.87	0.55
2:K:151:LEU:CG	2:K:151:LEU:O	2.54	0.55
3:P:7148:VAL:HG12	3:P:7168:THR:HA	1.88	0.55
1:C:175:ARG:HG3	1:C:175:ARG:NH1	2.22	0.55
1:N:232:ARG:HA	1:N:263:TRP:CZ2	2.42	0.55
1:E:111:ARG:CB	1:E:114:LEU:HD22	2.28	0.55
1:E:200:ASN:ND2	1:E:206:LYS:HE2	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:7135:ILE:HG21	3:P:7151:GLY:HA3	1.89	0.55
1:M:42:ILE:HG22	1:M:43:PRO:O	2.07	0.55
3:Q:5010:LEU:O	3:Q:5013:ASN:N	2.38	0.55
3:R:6116:THR:HG21	3:R:6147:ILE:HD11	1.88	0.55
1:L:49:SER:HB2	1:L:51:SER:O	2.07	0.55
6:L:700:08T:N3	6:L:700:08T:O2'	2.40	0.55
1:E:277:THR:HG23	1:E:280:SER:CB	2.36	0.55
1:M:48:HIS:NE2	1:M:156:THR:HB	2.22	0.55
1:C:57:THR:HG23	1:C:137:THR:HG21	1.89	0.55
1:E:85:ARG:O	1:E:89:THR:HB	2.07	0.55
2:K:127:LEU:HD13	2:K:141:TYR:HB3	1.89	0.55
1:B:232:ARG:HG3	1:B:233:GLY:N	2.21	0.55
1:L:238:VAL:HG22	1:L:253:LEU:HD13	1.88	0.55
3:Q:5001:MSE:N	3:Q:5072:GLU:OE2	2.40	0.55
1:D:201:PHE:O	1:D:202:PRO:C	2.44	0.55
1:E:3:THR:HG21	1:E:18:SER:HB2	1.88	0.55
1:B:186:ALA:HB3	1:B:219:VAL:CG2	2.36	0.55
1:O:67:VAL:HG12	1:O:67:VAL:O	2.07	0.55
2:A:80:TYR:CE1	2:A:84:LEU:HD11	2.42	0.55
1:C:297:ILE:HD13	1:D:297:ILE:CD1	2.26	0.55
1:D:97:PHE:CZ	3:G:5078:ASP:C	2.80	0.55
1:B:75:ASN:HB3	1:B:78:ASP:HB2	1.89	0.55
5:T:17:DC:H2'	5:T:18:DA:C8	2.42	0.55
3:G:5007:THR:HG23	3:G:5044:ILE:CG2	2.37	0.55
1:E:55:GLY:O	1:E:59:VAL:HG23	2.08	0.55
1:D:189:ASP:O	1:D:192:VAL:HG12	2.06	0.54
1:O:173:ILE:HG23	1:O:193:VAL:HG12	1.88	0.54
3:Q:5010:LEU:HD12	3:Q:5190:GLN:OE1	2.07	0.54
1:D:3:THR:OG1	1:D:18:SER:HB2	2.07	0.54
2:A:116:GLU:HG2	2:A:116:GLU:O	2.07	0.54
1:C:297:ILE:CG2	1:D:293:GLN:O	2.55	0.54
1:N:277:THR:HG23	1:N:280:SER:CB	2.37	0.54
1:O:81:ILE:HG23	1:O:82:ASP:OD1	2.07	0.54
2:K:41:PHE:HD2	4:S:9:DT:C7	2.18	0.54
3:R:6023:LEU:HD12	3:R:6023:LEU:O	2.07	0.54
3:P:7136:ASP:O	3:P:7137:THR:OG1	2.24	0.54
1:O:32:THR:O	1:O:36:ILE:HG13	2.07	0.54
1:B:201:PHE:O	1:B:202:PRO:C	2.39	0.54
1:L:289:GLY:C	2:K:85:ILE:HG23	2.27	0.54
1:B:293:GLN:OE1	2:A:85:ILE:CG1	2.56	0.54
2:K:183:LEU:O	2:K:187:TRP:CD1	2.61	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:700:08T:O1B	6:C:700:08T:F1	2.15	0.54
1:N:303:LEU:HD22	1:O:265:VAL:HG11	1.89	0.54
1:C:250:LEU:HD13	1:C:309:PHE:HB3	1.88	0.54
1:E:81:ILE:HG13	1:E:85:ARG:NH1	2.22	0.54
1:D:192:VAL:HG11	1:D:220:LEU:HB3	1.89	0.54
5:J:1:DG:H2"	5:J:2:DC:C5'	2.38	0.54
1:D:46:ILE:HB	1:D:154:VAL:HG22	1.90	0.54
3:Q:5112:ALA:HB2	3:Q:5197:LEU:HD22	1.88	0.54
1:B:289:GLY:HA3	2:A:85:ILE:CG2	2.38	0.54
1:C:169:MET:O	1:C:173:ILE:HG13	2.08	0.54
2:A:69:LEU:CD1	2:A:98:LEU:HD13	2.36	0.54
1:L:232:ARG:HG3	1:L:233:GLY:H	1.72	0.54
1:D:121:LEU:O	1:D:125:MET:HG3	2.07	0.54
1:B:279:GLN:O	1:B:282:ILE:HG22	2.07	0.54
1:D:297:ILE:HG22	1:E:295:HIS:O	2.08	0.54
1:B:293:GLN:NE2	1:E:297:ILE:HG22	2.23	0.54
1:L:48:HIS:CG	1:L:141:ILE:HG12	2.43	0.54
1:M:316:MET:HB3	1:M:318:TRP:CZ3	2.43	0.54
3:R:6035:ASN:OD1	3:R:6037:THR:CG2	2.53	0.54
1:O:56:LYS:HB3	1:O:137:THR:HG23	1.89	0.54
3:H:6067:VAL:HG12	3:H:6068:ASN:N	2.23	0.54
3:H:6183:ASN:O	3:H:6186:ASN:HB2	2.08	0.54
3:R:6056:ASP:OD2	3:R:6059:GLY:HA3	2.07	0.54
1:M:110:ASP:OD1	1:N:122:ARG:NH2	2.40	0.54
1:C:251:ARG:HH11	1:C:251:ARG:HG3	1.72	0.54
1:O:85:ARG:O	1:O:89:THR:HB	2.06	0.54
1:C:277:THR:HG23	1:C:280:SER:CB	2.38	0.54
3:H:6210:GLU:HA	3:H:6215:ASN:HD22	1.72	0.54
1:O:169:MET:O	1:O:173:ILE:HG13	2.07	0.54
1:O:238:VAL:HG22	1:O:253:LEU:HD13	1.90	0.54
1:C:220:LEU:HA	1:C:224:ILE:HD12	1.89	0.54
3:R:6092:TRP:HD1	3:R:6093:PRO:O	1.90	0.54
3:F:7190:GLN:O	3:F:7194:TYR:HE2	1.89	0.54
1:B:87:PRO:HA	1:B:90:ASN:HB2	1.89	0.54
3:P:7121:GLU:HA	3:P:7124:GLN:HB3	1.89	0.54
3:H:6181:ILE:HD12	3:H:6223:ASP:CB	2.38	0.54
1:C:251:ARG:CG	1:C:251:ARG:HH11	2.20	0.54
2:K:40:PHE:CD2	2:K:64:MET:HG3	2.43	0.54
1:O:121:LEU:HA	1:O:124:PHE:HB3	1.90	0.54
1:E:189:ASP:O	1:E:192:VAL:HG12	2.07	0.54
3:F:7060:PHE:CE1	3:F:7083:ILE:HD11	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:97:PHE:CZ	3:Q:5078:ASP:HA	2.43	0.54
1:N:16:ARG:NH2	6:N:700:08T:O2A	2.41	0.54
1:N:251:ARG:HG3	1:N:251:ARG:HH11	1.73	0.54
3:G:5023:LEU:CD1	3:G:5052:VAL:HG12	2.38	0.54
3:G:5189:MSE:HG2	3:G:5189:MSE:O	2.07	0.54
2:A:152:PRO:O	2:A:156:LYS:HB2	2.08	0.54
1:O:48:HIS:HB2	1:O:138:ALA:O	2.07	0.54
3:H:6092:TRP:CD1	3:H:6093:PRO:HD2	2.43	0.54
1:M:80:LYS:HB3	4:S:18:DT:OP2	2.08	0.54
3:R:6175:GLU:O	3:R:6176:ASN:ND2	2.41	0.54
2:A:164:ASP:O	2:A:167:LEU:HB2	2.08	0.53
1:L:307:TYR:CD1	1:M:289:GLY:HA3	2.43	0.53
1:N:48:HIS:NE2	1:N:156:THR:HB	2.23	0.53
1:D:303:LEU:HD22	1:E:265:VAL:HG12	1.88	0.53
1:O:243:LYS:HG2	1:O:318:TRP:NE1	2.23	0.53
3:Q:5115:VAL:HG22	3:Q:5197:LEU:HD23	1.90	0.53
1:M:251:ARG:HG3	1:M:251:ARG:HH11	1.73	0.53
3:P:7001:MSE:N	3:P:7072:GLU:HG3	2.23	0.53
3:P:7109:PHE:CD1	3:P:7110:PRO:CD	2.71	0.53
3:G:5057:LEU:O	3:G:5061:LEU:HG	2.08	0.53
1:D:282:ILE:O	1:D:286:GLU:HG3	2.09	0.53
5:J:11:DC:H2"	5:J:12:DG:C8	2.43	0.53
3:Q:5180:PHE:CE2	3:Q:5198:LEU:HB3	2.43	0.53
3:R:6080:ASN:OD1	3:R:6093:PRO:HA	2.08	0.53
1:L:273:TYR:CD1	1:L:281:ILE:HD13	2.43	0.53
1:E:162:ASP:O	1:E:166:ILE:HG13	2.08	0.53
1:M:277:THR:CG2	1:M:317:GLN:O	2.56	0.53
1:L:116:GLU:OE1	1:L:119:ARG:NH1	2.41	0.53
3:Q:5066:LEU:O	3:R:6125:GLN:HG3	2.08	0.53
3:P:7162:ARG:CG	3:P:7162:ARG:HH11	2.20	0.53
1:O:10:ILE:HD13	2:K:141:TYR:CD2	2.44	0.53
2:A:164:ASP:HA	2:A:167:LEU:CD1	2.19	0.53
1:C:273:TYR:CD1	1:C:281:ILE:HD13	2.44	0.53
3:F:7030:MSE:CE	3:F:7103:PRO:HB2	2.38	0.53
1:N:72:MET:HE3	1:N:91:PHE:CG	2.43	0.53
5:J:5:DA:H2"	5:J:6:DC:C6	2.43	0.53
5:T:3:DA:H2"	5:T:4:DG:C5'	2.36	0.53
1:B:277:THR:HG23	1:B:280:SER:CB	2.38	0.53
1:E:173:ILE:HG23	1:E:193:VAL:HG12	1.89	0.53
3:G:5056:ASP:O	3:G:5058:ASN:N	2.41	0.53
3:F:7141:THR:HG21	3:F:7179:ASN:OD1	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:250:LEU:HD13	1:N:309:PHE:HB3	1.89	0.53
3:G:5011:LEU:CB	3:G:5061:LEU:HD11	2.38	0.53
2:K:11:ASN:O	2:K:15:VAL:HG23	2.09	0.53
3:F:7150:ASN:HB3	3:F:7152:PHE:CZ	2.43	0.53
3:P:7189:MSE:HB2	3:P:7216:TYR:CE1	2.44	0.53
3:P:7028:PHE:HE2	3:P:7030:MSE:HE3	1.73	0.53
3:P:7138:ILE:HG22	3:P:7151:GLY:HA2	1.90	0.53
3:Q:5136:ASP:OD1	3:Q:5137:THR:HG23	2.09	0.53
1:D:20:ILE:HG22	1:D:66:ASP:OD2	2.08	0.53
1:D:76:GLY:N	1:D:107:ASP:O	2.41	0.53
1:N:49:SER:HB3	1:N:56:LYS:HZ2	1.72	0.53
3:R:6150:ASN:HB2	3:R:6152:PHE:CE1	2.43	0.53
1:N:290:GLU:HG2	1:N:294:TYR:HE2	1.74	0.53
1:M:260:ASP:O	1:M:260:ASP:OD1	2.27	0.53
1:L:289:GLY:HA3	2:K:85:ILE:HG21	1.90	0.53
3:F:7210:GLU:HA	3:F:7215:ASN:HD22	1.74	0.53
5:J:17:DC:H2"	5:J:18:DA:H5'	1.91	0.53
1:C:192:VAL:HG11	1:C:220:LEU:HB3	1.91	0.53
3:R:6123:LEU:CD2	3:R:6191:PRO:HA	2.39	0.53
1:C:77:SER:OG	1:D:120:HIS:HA	2.09	0.53
3:P:7007:THR:OG1	3:P:7046:ASP:OD2	2.22	0.53
3:H:6021:ILE:CG2	3:H:6057:LEU:HD13	2.39	0.53
3:R:6120:ALA:HB2	3:R:6192:GLY:C	2.29	0.53
1:L:251:ARG:HG3	1:L:251:ARG:HH11	1.74	0.53
3:Q:5112:ALA:CB	3:Q:5197:LEU:HD22	2.38	0.53
1:E:304:HIS:HB2	2:A:83:ASN:ND2	2.24	0.53
1:E:56:LYS:HB2	8:E:700:ADP:O1B	2.09	0.53
3:G:5007:THR:CG2	3:G:5044:ILE:HG21	2.38	0.53
1:C:119:ARG:O	1:C:122:ARG:HG2	2.09	0.53
1:M:165:LYS:HG2	1:M:169:MET:CE	2.39	0.53
3:P:7064:LEU:HD23	3:P:7083:ILE:HD13	1.89	0.53
1:M:83:PHE:O	1:M:87:PRO:HD2	2.09	0.53
1:N:5:ASN:O	1:N:7:LYS:N	2.41	0.53
1:C:297:ILE:CD1	1:D:297:ILE:HD11	2.27	0.52
2:K:183:LEU:O	2:K:187:TRP:NE1	2.41	0.52
2:A:102:VAL:CG2	2:A:104:ARG:HH21	2.21	0.52
1:O:15:TYR:CE2	1:O:179:ILE:HG23	2.44	0.52
1:D:165:LYS:HG2	1:D:169:MET:CE	2.39	0.52
1:M:169:MET:O	1:M:173:ILE:HG13	2.09	0.52
1:C:68:ASN:O	1:C:100:ARG:HD3	2.09	0.52
1:D:301:THR:HG21	1:E:142:ASP:OD2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:5023:LEU:HD12	3:Q:5023:LEU:O	2.09	0.52
1:O:303:LEU:HD11	2:K:76:MET:HE1	1.89	0.52
2:A:7:ASP:OD2	3:F:7032:ARG:CZ	2.58	0.52
3:R:6208:LYS:HA	3:R:6217:VAL:HG22	1.91	0.52
3:G:5060:PHE:HB2	3:G:5092:TRP:CE2	2.44	0.52
3:Q:5180:PHE:CD2	3:Q:5198:LEU:HD13	2.44	0.52
1:C:201:PHE:O	1:C:202:PRO:C	2.47	0.52
3:Q:5063:ILE:HG12	3:Q:5092:TRP:HZ3	1.74	0.52
1:D:273:TYR:CD1	1:D:281:ILE:HD13	2.43	0.52
1:N:77:SER:HA	1:N:114:LEU:HD11	1.90	0.52
4:I:15:DT:H3	5:J:16:DA:H61	1.55	0.52
1:D:16:ARG:HB2	6:D:700:08T:O3'	2.09	0.52
1:C:97:PHE:O	3:G:5204:GLN:CB	2.57	0.52
1:B:292:ASN:HD21	2:A:88:GLY:HA3	1.72	0.52
1:M:71:MET:HE1	1:M:73:PHE:HD1	1.73	0.52
1:O:189:ASP:O	1:O:192:VAL:HG12	2.08	0.52
3:H:6039:TYR:CE2	3:H:6107:ILE:HG23	2.44	0.52
1:O:12:GLU:OE1	1:O:205:ARG:HD2	2.09	0.52
1:M:17:PRO:HB3	1:M:22:GLU:HB3	1.91	0.52
1:C:91:PHE:CE1	1:C:102:LYS:HD3	2.44	0.52
3:F:7139:ALA:HA	3:F:7180:PHE:O	2.09	0.52
1:E:67:VAL:HG12	1:E:67:VAL:O	2.08	0.52
1:C:303:LEU:CD2	1:D:265:VAL:CG1	2.82	0.52
1:L:81:ILE:O	1:L:85:ARG:HG3	2.09	0.52
2:A:40:PHE:CD2	2:A:64:MET:HG3	2.45	0.52
1:D:3:THR:HG21	1:D:18:SER:HB2	1.92	0.52
2:A:151:LEU:CG	2:A:151:LEU:O	2.57	0.52
3:F:7005:LYS:CG	3:F:7006:ASP:N	2.72	0.52
3:P:7122:ASP:HB3	3:P:7167:LEU:CD2	2.39	0.52
3:Q:5118:ILE:CD1	3:Q:5123:LEU:HB2	2.38	0.52
3:F:7054:ILE:CG2	3:F:7055:TYR:H	2.22	0.52
3:F:7146:LYS:HG2	3:F:7171:ASP:HA	1.91	0.52
1:M:251:ARG:CG	1:M:251:ARG:HH11	2.22	0.52
1:M:77:SER:HA	1:M:114:LEU:HD11	1.92	0.52
1:M:56:LYS:NZ	6:M:700:08T:O2B	2.34	0.52
1:N:119:ARG:O	1:N:122:ARG:HG2	2.09	0.52
1:M:97:PHE:HB2	3:Q:5205:GLY:O	2.09	0.52
3:P:7018:ASN:OD1	3:P:7019:SER:N	2.42	0.52
1:N:175:ARG:HG3	1:N:175:ARG:NH1	2.22	0.52
3:G:5109:PHE:CD1	3:G:5208:LYS:HD2	2.45	0.52
3:P:7042:ALA:HB2	3:P:7214:ALA:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:232:ARG:HA	1:N:263:TRP:HZ2	1.75	0.52
3:R:6210:GLU:CG	3:R:6215:ASN:HD21	2.22	0.52
3:R:6059:GLY:C	3:R:6092:TRP:CH2	2.83	0.52
1:L:67:VAL:O	1:L:67:VAL:HG12	2.09	0.52
1:B:273:TYR:CD1	1:B:281:ILE:HD13	2.45	0.52
1:O:307:TYR:CD2	2:K:80:TYR:CD1	2.97	0.52
3:H:6149:ILE:HD11	3:H:6169:LEU:HD11	1.92	0.52
1:B:276:VAL:CG2	1:B:318:TRP:HE3	2.22	0.52
3:R:6066:LEU:HD12	3:R:6067:VAL:N	2.25	0.52
1:O:111:ARG:CB	1:O:114:LEU:HD22	2.29	0.52
1:D:251:ARG:HH11	1:D:251:ARG:HG3	1.74	0.52
2:A:120:GLU:HG3	2:A:142:LYS:NZ	2.25	0.52
3:Q:5150:ASN:HA	3:Q:5165:TYR:O	2.10	0.52
3:R:6049:ASP:OD1	3:R:6050:PHE:CD1	2.62	0.52
1:B:71:MET:CE	1:B:105:VAL:HG21	2.40	0.52
1:C:80:LYS:HB3	4:I:18:DT:P	2.49	0.52
3:F:7182:ILE:HD13	3:F:7218:VAL:HG21	1.91	0.52
1:O:162:ASP:O	1:O:166:ILE:HG13	2.10	0.52
1:N:46:ILE:HB	1:N:154:VAL:HG22	1.91	0.52
1:D:290:GLU:HG2	1:D:294:TYR:HE2	1.75	0.52
1:M:48:HIS:CE1	1:M:141:ILE:CD1	2.86	0.52
3:G:5023:LEU:HD12	3:G:5023:LEU:O	2.10	0.52
3:R:6011:LEU:O	3:R:6057:LEU:HD21	2.09	0.52
3:H:6171:ASP:OD1	3:H:6171:ASP:N	2.42	0.52
3:F:7208:LYS:HA	3:F:7216:TYR:O	2.09	0.52
3:Q:5039:TYR:CD1	3:Q:5217:VAL:HG23	2.41	0.52
2:K:14:GLN:HB3	2:K:18:TYR:CE2	2.45	0.52
1:B:285:TYR:HD2	2:A:97:TYR:HB2	1.74	0.52
3:F:7147:ILE:HG12	3:F:7172:TYR:HB2	1.91	0.52
3:F:7110:PRO:HB2	3:F:7199:TRP:CD1	2.45	0.52
1:L:57:THR:CG2	1:L:107:ASP:OD1	2.57	0.51
1:B:251:ARG:HH11	1:B:251:ARG:CG	2.24	0.51
1:N:96:SER:HB2	1:N:102:LYS:HE2	1.93	0.51
1:O:96:SER:HB2	1:O:98:ASP:OD1	2.10	0.51
1:M:85:ARG:O	1:M:89:THR:HB	2.10	0.51
1:D:170:LYS:HZ1	1:N:39:LYS:CG	2.24	0.51
4:S:9:DT:H2"	4:S:10:DT:OP2	2.09	0.51
1:O:243:LYS:HG2	1:O:318:TRP:CE2	2.45	0.51
3:P:7030:MSE:HE2	3:P:7106:PRO:HB3	1.91	0.51
3:R:6055:TYR:HB2	3:R:6095:ALA:HB2	1.93	0.51
1:E:56:LYS:HB3	1:E:137:THR:HG23	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:5113:SER:HB2	3:G:5199:TRP:HA	1.92	0.51
1:D:175:ARG:HG3	1:D:175:ARG:NH1	2.24	0.51
1:N:29:ASP:O	1:N:32:THR:HG22	2.10	0.51
2:K:161:LEU:HD12	2:K:163:THR:HG23	1.91	0.51
1:O:83:PHE:HE1	1:O:87:PRO:HG2	1.76	0.51
3:P:7202:GLY:C	3:P:7204:GLN:H	2.11	0.51
1:N:303:LEU:HD22	1:O:265:VAL:HG12	1.92	0.51
3:R:6023:LEU:HD13	3:R:6048:ILE:HD13	1.92	0.51
4:S:25:DG:H1'	4:S:26:DT:H5'	1.91	0.51
1:N:230:ASN:CG	1:N:231:ASP:HA	2.31	0.51
1:N:85:ARG:O	1:N:89:THR:HB	2.10	0.51
1:N:251:ARG:HH21	1:O:270:GLU:HA	1.73	0.51
1:O:288:VAL:HG22	1:O:308:LEU:HD11	1.93	0.51
2:A:152:PRO:O	2:A:156:LYS:N	2.43	0.51
1:N:35:SER:O	1:N:38:SER:HB2	2.11	0.51
1:E:238:VAL:HG22	1:E:253:LEU:HD13	1.92	0.51
3:Q:5189:MSE:CB	3:Q:5216:TYR:CE2	2.94	0.51
1:M:238:VAL:HG22	1:M:253:LEU:HD13	1.92	0.51
1:B:251:ARG:HD2	1:C:285:TYR:OH	2.10	0.51
3:P:7060:PHE:CE2	3:P:7064:LEU:HD11	2.45	0.51
3:P:7202:GLY:C	3:P:7204:GLN:N	2.64	0.51
1:M:273:TYR:CD1	1:M:281:ILE:HD13	2.45	0.51
1:O:303:LEU:HD21	2:K:79:VAL:HG12	1.93	0.51
4:S:10:DT:OP2	4:S:10:DT:C6	2.63	0.51
1:O:200:ASN:ND2	1:O:206:LYS:HE2	2.26	0.51
1:B:5:ASN:C	1:B:7:LYS:H	2.12	0.51
1:N:121:LEU:O	1:N:125:MET:HG3	2.11	0.51
3:H:6195:LYS:HD2	3:H:6197:LEU:HD21	1.92	0.51
1:N:271:GLU:O	1:N:275:ARG:HD2	2.10	0.51
3:F:7007:THR:OG1	3:F:7046:ASP:OD2	2.16	0.51
1:D:55:GLY:O	1:D:59:VAL:HG23	2.10	0.51
3:Q:5018:ASN:HB3	3:Q:5031:THR:OG1	2.11	0.51
1:O:290:GLU:HG2	1:O:294:TYR:HE2	1.76	0.51
3:F:7004:SER:HB3	3:F:7046:ASP:OD2	2.11	0.51
1:E:14:LYS:HE2	1:E:15:TYR:CE1	2.46	0.51
1:B:238:VAL:O	1:B:242:LEU:HD13	2.11	0.51
3:G:5037:THR:CG2	3:G:5186:ASN:CG	2.79	0.51
3:H:6050:PHE:CD1	3:H:6050:PHE:N	2.78	0.51
1:D:277:THR:HG23	1:D:280:SER:CB	2.40	0.51
2:A:183:LEU:O	2:A:187:TRP:NE1	2.43	0.51
1:B:276:VAL:HG23	1:B:317:GLN:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:7114:ALA:HB3	3:P:7198:LEU:HB2	1.93	0.51
3:P:7139:ALA:HA	3:P:7180:PHE:O	2.11	0.51
1:N:204:PHE:O	1:N:207:THR:HG22	2.10	0.51
1:O:55:GLY:O	1:O:59:VAL:HG23	2.10	0.51
1:D:57:THR:OG1	6:D:700:08T:O1B	2.09	0.51
1:L:48:HIS:CE1	1:L:141:ILE:CD1	2.89	0.51
1:L:271:GLU:O	1:L:275:ARG:HD2	2.10	0.51
3:R:6027:GLN:HB3	3:R:6044:ILE:O	2.11	0.51
1:D:310:ILE:HG12	1:E:285:TYR:CD2	2.39	0.51
3:R:6130:SER:CB	3:R:6135:ILE:HB	2.40	0.51
1:E:57:THR:CG2	1:E:107:ASP:OD1	2.58	0.51
1:D:213:SER:CB	1:E:153:ARG:CZ	2.89	0.51
1:E:165:LYS:HG2	1:E:169:MET:HE3	1.92	0.51
1:B:251:ARG:HH11	1:B:251:ARG:HG3	1.75	0.51
1:O:33:PHE:CZ	1:O:59:VAL:HG11	2.45	0.51
1:E:113:GLY:HA3	4:I:13:DT:H5"	1.92	0.50
1:M:204:PHE:HB2	6:M:700:08T:C8	2.41	0.50
4:S:8:DT:H2"	4:S:9:DT:H5'	1.93	0.50
5:T:3:DA:C6	5:T:4:DG:C6	2.99	0.50
2:K:120:GLU:HG3	2:K:142:LYS:NZ	2.26	0.50
5:J:9:DT:C2'	5:J:10:DA:OP2	2.59	0.50
3:Q:5119:LYS:O	3:Q:5122:ASP:HB2	2.11	0.50
1:D:238:VAL:HG22	1:D:253:LEU:HD13	1.93	0.50
1:B:185:ILE:HD13	1:B:215:SER:HB2	1.91	0.50
3:F:7023:LEU:C	3:F:7023:LEU:HD12	2.31	0.50
2:K:85:ILE:HG22	2:K:89:LEU:CD1	2.42	0.50
2:A:85:ILE:HG22	2:A:89:LEU:HD11	1.92	0.50
1:M:16:ARG:NH2	6:M:700:08T:O2A	2.44	0.50
3:F:7028:PHE:HE1	3:F:7041:GLU:HB2	1.76	0.50
1:O:277:THR:HG23	1:O:280:SER:CB	2.39	0.50
3:R:6178:PHE:HD2	3:R:6180:PHE:CD2	2.29	0.50
4:I:29:DG:O5'	4:I:29:DG:C2'	2.60	0.50
3:P:7022:MSE:CE	3:P:7024:LYS:HG3	2.39	0.50
1:L:238:VAL:O	1:L:242:LEU:HD13	2.12	0.50
3:G:5165:TYR:HD1	3:F:7090:ILE:CG1	2.24	0.50
1:D:85:ARG:O	1:D:89:THR:HB	2.12	0.50
1:D:116:GLU:OE2	1:D:119:ARG:NH1	2.45	0.50
1:N:251:ARG:CG	1:N:251:ARG:HH11	2.23	0.50
1:B:121:LEU:O	1:B:125:MET:HG3	2.10	0.50
2:K:152:PRO:O	2:K:156:LYS:HB2	2.11	0.50
2:A:109:GLY:HA2	4:I:8:DT:H1'	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:7134:GLN:O	3:P:7153:ASN:HB2	2.11	0.50
3:P:7076:SER:HB3	3:P:7080:ASN:O	2.11	0.50
3:P:7001:MSE:HB3	3:P:7049:ASP:OD2	2.10	0.50
1:D:254:ALA:N	1:D:255:PRO:HD2	2.26	0.50
3:G:5087:ARG:HH12	3:H:6119:LYS:CD	2.12	0.50
1:O:303:LEU:HD11	2:K:76:MET:CE	2.42	0.50
1:D:170:LYS:CE	1:N:39:LYS:HA	2.39	0.50
3:G:5021:ILE:HG22	3:G:5057:LEU:HD13	1.93	0.50
3:R:6076:SER:N	3:R:6080:ASN:O	2.42	0.50
1:C:282:ILE:O	1:C:286:GLU:HG3	2.11	0.50
3:P:7120:ALA:CB	3:P:7193:ASN:OD1	2.60	0.50
1:O:253:LEU:HD23	2:K:114:LEU:HD11	1.93	0.50
1:O:204:PHE:O	1:O:207:THR:HG22	2.12	0.50
3:G:5163:VAL:HG22	3:G:5163:VAL:O	2.12	0.50
1:N:97:PHE:CE2	3:Q:5079:GLY:N	2.72	0.50
1:M:57:THR:HG23	1:M:137:THR:HG21	1.92	0.50
1:E:276:VAL:HG23	1:E:318:TRP:HB3	1.92	0.50
1:D:119:ARG:O	1:D:122:ARG:HG2	2.12	0.50
1:L:243:LYS:HG2	1:L:318:TRP:NE1	2.26	0.50
1:D:97:PHE:CE1	3:G:5078:ASP:O	2.65	0.50
5:J:9:DT:C2'	5:J:10:DA:H5'	2.40	0.50
2:A:162:VAL:O	2:A:162:VAL:CG1	2.59	0.50
1:L:251:ARG:HH11	1:L:251:ARG:CG	2.24	0.50
1:B:247:VAL:O	1:B:248:LYS:C	2.50	0.50
1:D:48:HIS:CE1	1:D:141:ILE:CD1	2.85	0.50
1:O:219:VAL:CG1	1:O:220:LEU:N	2.75	0.50
3:P:7089:THR:CG2	3:P:7091:PHE:CE1	2.95	0.50
1:E:83:PHE:HE1	1:E:87:PRO:HG2	1.76	0.50
1:O:33:PHE:CE2	1:O:59:VAL:HG11	2.46	0.50
2:K:152:PRO:O	2:K:156:LYS:N	2.44	0.50
1:L:292:ASN:ND2	2:K:88:GLY:CA	2.71	0.50
3:G:5113:SER:HB3	3:G:5228:PHE:CE1	2.47	0.50
3:R:6071:ALA:O	3:R:6073:ILE:HG13	2.12	0.50
3:F:7178:PHE:HB3	3:F:7226:HIS:ND1	2.27	0.50
1:L:5:ASN:O	1:L:7:LYS:N	2.45	0.50
1:E:96:SER:HB2	1:E:98:ASP:OD1	2.12	0.50
1:B:235:ILE:O	1:B:235:ILE:HG22	2.11	0.50
2:K:55:ILE:CG1	2:K:56:ALA:N	2.68	0.50
4:I:17:DC:N4	5:J:14:DG:H22	2.10	0.50
1:B:299:ALA:HB2	1:C:295:HIS:HD2	1.76	0.50
3:R:6178:PHE:HB2	3:R:6180:PHE:CE2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:125:MET:O	1:B:129:SER:HB2	2.11	0.50
2:A:109:GLY:HA3	4:I:8:DT:C4'	2.42	0.50
1:L:80:LYS:HB3	4:S:20:DG:OP2	2.10	0.50
1:C:122:ARG:HG2	1:C:122:ARG:HH11	1.77	0.50
1:B:161:THR:HG23	1:B:164:ASP:OD2	2.11	0.50
1:M:230:ASN:C	1:M:230:ASN:OD1	2.50	0.50
1:N:288:VAL:HG22	1:N:308:LEU:HD11	1.93	0.50
1:D:5:ASN:O	1:D:7:LYS:N	2.44	0.50
1:M:8:GLU:OE2	1:M:13:GLN:HB3	2.11	0.50
1:L:8:GLU:OE2	1:L:13:GLN:HB3	2.12	0.50
3:Q:5140:ILE:HG13	3:Q:5148:VAL:O	2.12	0.50
1:B:20:ILE:HD13	1:B:63:LEU:HD23	1.92	0.50
2:K:130:ARG:HD2	2:K:130:ARG:O	2.12	0.50
1:L:277:THR:CG2	1:L:317:GLN:O	2.56	0.49
3:F:7210:GLU:HG3	3:F:7215:ASN:HD21	1.76	0.49
3:P:7135:ILE:HA	3:P:7152:PHE:O	2.12	0.49
3:Q:5028:PHE:HA	3:Q:5042:ALA:O	2.12	0.49
3:P:7089:THR:HG22	3:P:7091:PHE:HE1	1.75	0.49
1:O:3:THR:OG1	1:O:22:GLU:OE1	2.30	0.49
1:C:96:SER:HB2	1:C:102:LYS:HE2	1.94	0.49
3:G:5082:LYS:HB2	3:G:5091:PHE:HE1	1.76	0.49
1:L:186:ALA:HB3	1:L:219:VAL:CG2	2.42	0.49
3:H:6063:ILE:HD13	3:F:7129:VAL:HG22	1.94	0.49
1:O:64:CYS:SG	1:O:103:VAL:HG11	2.52	0.49
1:N:256:LYS:HD2	1:O:159:GLN:HE22	1.76	0.49
1:C:260:ASP:OD1	1:C:260:ASP:O	2.29	0.49
1:D:170:LYS:NZ	1:N:39:LYS:N	2.53	0.49
3:R:6178:PHE:HD2	3:R:6180:PHE:CE2	2.25	0.49
1:E:175:ARG:O	1:E:179:ILE:HG13	2.12	0.49
2:A:11:ASN:O	2:A:15:VAL:HG23	2.12	0.49
1:O:243:LYS:HG2	1:O:318:TRP:HE1	1.77	0.49
1:L:161:THR:HG23	1:L:164:ASP:OD2	2.12	0.49
1:E:247:VAL:O	1:E:248:LYS:C	2.49	0.49
3:F:7032:ARG:HB3	3:F:7103:PRO:HG3	1.93	0.49
1:B:303:LEU:HD22	1:C:265:VAL:HG12	1.91	0.49
2:K:116:GLU:O	2:K:116:GLU:HG2	2.12	0.49
1:L:289:GLY:CA	2:K:85:ILE:HG23	2.42	0.49
1:D:48:HIS:NE2	1:D:156:THR:HB	2.26	0.49
3:Q:5201:LYS:O	3:Q:5204:GLN:HB2	2.12	0.49
3:H:6039:TYR:CE2	3:H:6107:ILE:CG2	2.95	0.49
1:O:14:LYS:HE2	1:O:15:TYR:CE1	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:277:THR:HG23	1:L:280:SER:CB	2.41	0.49
5:T:3:DA:H2"	5:T:4:DG:OP2	2.13	0.49
3:P:7152:PHE:CD2	3:P:7160:LEU:HD22	2.47	0.49
3:Q:5189:MSE:O	3:Q:5189:MSE:HG2	2.12	0.49
1:E:165:LYS:O	1:E:169:MET:HG3	2.12	0.49
1:D:38:SER:O	1:D:40:GLY:N	2.45	0.49
1:M:9:HIS:CD2	1:N:41:LYS:HB3	2.47	0.49
1:N:151:ARG:HH11	1:N:151:ARG:HG3	1.77	0.49
1:O:251:ARG:CG	1:O:251:ARG:NH1	2.75	0.49
1:C:116:GLU:OE2	1:C:119:ARG:NH1	2.45	0.49
1:L:303:LEU:HD22	1:M:265:VAL:HG12	1.94	0.49
3:H:6016:THR:O	3:H:6188:LYS:HD3	2.12	0.49
1:M:165:LYS:HG2	1:M:169:MET:HE1	1.93	0.49
1:E:141:ILE:O	1:E:143:GLY:N	2.46	0.49
3:R:6092:TRP:CD1	3:R:6093:PRO:O	2.66	0.49
3:P:7189:MSE:HE2	3:P:7209:PHE:CD2	2.48	0.49
1:E:121:LEU:HA	1:E:124:PHE:HB3	1.93	0.49
1:B:200:ASN:OD1	1:B:200:ASN:N	2.45	0.49
1:L:293:GLN:HE22	1:O:297:ILE:HG22	1.75	0.49
3:R:6138:ILE:HG23	3:R:6184:MSE:HE3	1.93	0.49
3:R:6149:ILE:HD12	3:R:6167:LEU:HD23	1.95	0.49
1:D:169:MET:O	1:D:173:ILE:HG13	2.12	0.49
1:E:81:ILE:HG22	4:I:14:DG:P	2.53	0.49
3:H:6181:ILE:HD12	3:H:6223:ASP:HB2	1.94	0.49
3:H:6120:ALA:CB	3:H:6192:GLY:HA2	2.42	0.49
2:A:105:GLY:O	2:A:106:LYS:HB2	2.12	0.49
3:F:7220:LEU:HD23	3:F:7220:LEU:N	2.28	0.49
6:D:700:08T:N3	6:D:700:08T:C2'	2.71	0.49
3:H:6103:PRO:O	3:H:6104:ASN:HB3	2.12	0.49
3:P:7118:ILE:CG1	3:P:7119:LYS:N	2.67	0.49
3:R:6032:ARG:HG2	3:R:6103:PRO:HB3	1.94	0.49
1:B:186:ALA:HB3	1:B:219:VAL:HG22	1.93	0.49
1:B:288:VAL:HG22	1:B:308:LEU:HD11	1.95	0.49
1:C:75:ASN:ND2	1:D:123:SER:HB3	2.28	0.49
3:Q:5113:SER:OG	3:Q:5199:TRP:HA	2.12	0.49
1:E:132:CYS:SG	1:E:133:SER:N	2.85	0.49
1:O:2:ILE:HD12	1:O:178:GLU:HG2	1.94	0.49
1:C:251:ARG:NH2	1:D:270:GLU:CG	2.73	0.49
2:K:4:PHE:CZ	3:P:7039:TYR:HD2	2.31	0.49
1:L:276:VAL:HA	1:L:318:TRP:HB3	1.94	0.49
3:R:6008:THR:O	3:R:6011:LEU:HB2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:7082:LYS:HE3	3:P:7089:THR:HG21	1.95	0.49
1:E:263:TRP:CZ3	2:A:136:ASN:ND2	2.80	0.49
3:G:5139:ALA:HA	3:G:5180:PHE:O	2.12	0.49
1:E:21:ASP:O	1:E:30:LYS:NZ	2.45	0.49
1:E:271:GLU:O	1:E:275:ARG:HD2	2.13	0.49
1:D:291:ASN:ND2	1:D:304:HIS:CE1	2.81	0.49
3:R:6157:ASP:OD1	3:R:6161:THR:HB	2.13	0.49
1:E:109:PHE:CE2	1:E:118:GLN:HG2	2.47	0.49
1:D:96:SER:HB2	1:D:102:LYS:HE2	1.95	0.49
1:M:277:THR:HG23	1:M:280:SER:CB	2.41	0.49
3:R:6150:ASN:HB2	3:R:6152:PHE:HE1	1.78	0.49
1:M:29:ASP:CA	1:M:32:THR:HG22	2.42	0.49
1:N:165:LYS:HG2	1:N:169:MET:HE2	1.94	0.49
1:E:33:PHE:CE2	1:E:59:VAL:HG11	2.48	0.49
3:F:7113:SER:HB2	3:F:7198:LEU:O	2.13	0.49
2:A:3:LEU:HB2	2:A:4:PHE:CD2	2.48	0.49
3:P:7018:ASN:HB2	3:P:7032:ARG:O	2.13	0.49
1:D:303:LEU:HD21	1:E:288:VAL:HG12	1.95	0.49
1:E:213:SER:HA	2:A:148:ASN:HD22	1.77	0.49
3:G:5200:ALA:CB	3:G:5226:HIS:CD2	2.96	0.49
1:B:12:GLU:HA	1:B:208:ILE:HG21	1.95	0.49
1:B:8:GLU:OE2	1:B:13:GLN:HB3	2.12	0.49
1:D:260:ASP:OD1	1:D:260:ASP:O	2.31	0.49
3:H:6066:LEU:N	3:H:6066:LEU:HD23	2.28	0.49
2:A:6:ASP:OD1	2:A:6:ASP:O	2.31	0.49
3:Q:5128:ARG:CD	3:P:7066:LEU:HD22	2.31	0.48
1:B:293:GLN:OE1	2:A:85:ILE:HG12	2.13	0.48
1:E:219:VAL:CG1	1:E:220:LEU:N	2.76	0.48
3:G:5027:GLN:O	3:G:5044:ILE:HG13	2.13	0.48
3:Q:5008:THR:HA	3:Q:5011:LEU:HD13	1.95	0.48
1:M:116:GLU:OE2	1:M:119:ARG:NH1	2.46	0.48
1:C:8:GLU:OE2	1:C:13:GLN:HB3	2.13	0.48
1:E:24:ILE:HG22	1:E:168:MET:HE3	1.95	0.48
1:D:93:SER:HA	3:G:5099:THR:HG21	1.95	0.48
1:D:75:ASN:HB3	1:D:78:ASP:HB2	1.93	0.48
1:O:247:VAL:O	1:O:248:LYS:C	2.51	0.48
1:N:273:TYR:CD1	1:N:281:ILE:HD13	2.48	0.48
1:C:297:ILE:HG22	1:D:293:GLN:O	2.12	0.48
1:M:204:PHE:O	1:M:207:THR:HG22	2.13	0.48
1:E:16:ARG:NH2	8:E:700:ADP:H5'2	2.27	0.48
1:C:275:ARG:O	1:C:318:TRP:CD1	2.66	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:80:LYS:HB3	4:S:18:DT:P	2.52	0.48
1:L:162:ASP:O	1:L:166:ILE:HG13	2.13	0.48
3:F:7012:LYS:O	3:F:7015:ALA:HB3	2.12	0.48
2:A:154:VAL:O	2:A:158:LEU:HG	2.12	0.48
1:L:293:GLN:HE22	1:O:297:ILE:CG2	2.26	0.48
1:D:316:MET:HB3	1:D:318:TRP:CZ3	2.48	0.48
1:C:111:ARG:HH22	4:I:17:DC:P	2.37	0.48
3:F:7022:MSE:HE1	3:F:7024:LYS:HD3	1.95	0.48
3:H:6113:SER:O	3:H:6228:PHE:HE2	1.96	0.48
3:H:6227:ASP:O	3:H:6227:ASP:OD1	2.30	0.48
1:B:190:MET:C	1:B:192:VAL:N	2.66	0.48
4:S:24:DT:H3	5:T:7:DA:N6	2.10	0.48
1:M:158:GLY:C	1:M:160:PRO:HD3	2.33	0.48
1:B:254:ALA:N	1:B:255:PRO:HD2	2.28	0.48
1:L:293:GLN:OE1	2:K:85:ILE:HG13	2.13	0.48
1:B:293:GLN:OE1	2:A:85:ILE:HG13	2.13	0.48
1:L:48:HIS:HA	1:L:138:ALA:O	2.13	0.48
3:R:6037:THR:HG23	3:R:6038:THR:HB	1.94	0.48
3:R:6071:ALA:HA	3:R:6084:ALA:O	2.13	0.48
3:R:6066:LEU:HD11	3:R:6090:ILE:CD1	2.44	0.48
1:O:141:ILE:O	1:O:144:ILE:N	2.44	0.48
1:C:224:ILE:O	1:C:228:VAL:HG23	2.13	0.48
3:G:5114:ALA:HB3	3:G:5198:LEU:HD11	1.96	0.48
5:J:1:DG:H2"	5:J:2:DC:H5'	1.96	0.48
1:M:271:GLU:O	1:M:275:ARG:HD2	2.14	0.48
1:E:254:ALA:N	1:E:255:PRO:HD2	2.28	0.48
1:L:87:PRO:HA	1:L:90:ASN:HB2	1.95	0.48
3:R:6118:ILE:O	3:R:6118:ILE:HG23	2.14	0.48
3:H:6221:GLU:HA	3:H:6221:GLU:OE1	2.13	0.48
1:D:299:ALA:HB3	1:E:292:ASN:OD1	2.13	0.48
1:L:247:VAL:O	1:L:248:LYS:C	2.52	0.48
1:M:282:ILE:O	1:M:286:GLU:HG3	2.12	0.48
6:D:700:08T:N3	6:D:700:08T:H6	2.28	0.48
1:E:217:LYS:HG3	1:E:219:VAL:H	1.77	0.48
1:B:299:ALA:HB1	1:C:262:SER:CB	2.35	0.48
4:S:25:DG:H5'	4:S:25:DG:H8	1.78	0.48
1:D:246:ASP:OD1	1:D:246:ASP:N	2.46	0.48
3:Q:5136:ASP:CG	3:Q:5154:LYS:H	2.17	0.48
1:C:67:VAL:O	1:C:67:VAL:CG1	2.60	0.48
1:L:242:LEU:CD1	1:L:250:LEU:HD21	2.42	0.48
3:Q:5189:MSE:HE2	3:Q:5209:PHE:CG	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:7089:THR:CG2	3:P:7091:PHE:HE1	2.26	0.48
1:C:200:ASN:HD21	1:C:210:GLU:HG3	1.78	0.48
1:M:46:ILE:HB	1:M:154:VAL:HG22	1.95	0.48
3:Q:5220:LEU:HD23	3:Q:5220:LEU:N	2.29	0.48
1:L:293:GLN:OE1	2:K:85:ILE:CG1	2.61	0.48
1:B:260:ASP:O	1:B:260:ASP:OD1	2.31	0.48
1:L:275:ARG:O	1:L:318:TRP:CD1	2.67	0.48
3:P:7113:SER:HB3	3:P:7228:PHE:CZ	2.48	0.48
3:R:6149:ILE:HD11	3:R:6169:LEU:HD11	1.96	0.48
1:C:276:VAL:HG23	1:C:317:GLN:O	2.14	0.48
3:G:5201:LYS:HD3	3:G:5204:GLN:NE2	2.29	0.48
3:P:7120:ALA:N	3:P:7193:ASN:OD1	2.47	0.48
1:M:201:PHE:O	1:M:202:PRO:C	2.48	0.48
1:N:294:TYR:CD2	1:O:293:GLN:NE2	2.81	0.48
1:M:91:PHE:CE1	1:M:102:LYS:HD3	2.48	0.48
1:N:75:ASN:HB3	1:N:78:ASP:HB2	1.95	0.48
1:N:256:LYS:CD	1:O:159:GLN:NE2	2.75	0.48
3:F:7133:LEU:HB3	3:F:7164:LYS:NZ	2.29	0.48
1:E:251:ARG:NE	2:A:71:GLN:CD	2.56	0.48
3:P:7190:GLN:O	3:P:7194:TYR:OH	2.17	0.48
3:H:6156:GLU:O	3:H:6162:ARG:NH2	2.46	0.48
3:R:6011:LEU:HB3	3:R:6061:LEU:HD21	1.95	0.48
1:M:29:ASP:O	1:M:32:THR:HG22	2.14	0.48
1:M:47:LEU:HD22	1:M:157:PHE:CE1	2.48	0.48
1:C:201:PHE:HB3	1:C:202:PRO:HD3	1.96	0.48
3:G:5039:TYR:OH	3:G:5106:PRO:HA	2.13	0.48
1:L:291:ASN:ND2	1:L:304:HIS:CE1	2.81	0.48
1:M:75:ASN:HB3	1:M:78:ASP:HB2	1.95	0.48
1:N:68:ASN:O	1:N:100:ARG:HD3	2.14	0.48
1:O:213:SER:C	2:K:148:ASN:ND2	2.64	0.48
1:M:303:LEU:HD22	1:N:265:VAL:HG11	1.94	0.48
1:D:214:TYR:O	1:D:224:ILE:HD13	2.14	0.48
2:K:19:SER:HB3	3:P:7034:VAL:HG21	1.96	0.48
1:O:276:VAL:HA	1:O:318:TRP:HB3	1.95	0.48
3:Q:5025:SER:HA	3:Q:5048:ILE:HG22	1.96	0.48
1:N:235:ILE:HG22	1:N:235:ILE:O	2.14	0.48
1:C:5:ASN:O	1:C:7:LYS:N	2.46	0.48
2:A:167:LEU:CD1	2:A:180:LEU:HG	2.44	0.48
3:R:6055:TYR:CD1	3:R:6055:TYR:O	2.67	0.48
1:N:5:ASN:C	1:N:7:LYS:H	2.16	0.48
1:N:201:PHE:O	1:N:202:PRO:C	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:235:ILE:O	1:L:235:ILE:HG22	2.14	0.48
4:I:23:DG:O5'	4:I:23:DG:H2'	2.13	0.48
3:Q:5210:GLU:CA	3:Q:5215:ASN:ND2	2.66	0.48
1:N:76:GLY:N	1:N:107:ASP:O	2.46	0.48
3:R:6052:VAL:HG21	3:R:6081:ILE:HD11	1.95	0.48
1:E:12:GLU:OE1	1:E:205:ARG:HG3	2.14	0.48
1:O:201:PHE:O	1:O:202:PRO:C	2.49	0.48
3:R:6050:PHE:CD1	3:R:6050:PHE:N	2.82	0.48
2:A:63:PHE:O	2:A:67:ASN:HB2	2.13	0.48
2:K:164:ASP:HA	2:K:167:LEU:CD1	2.16	0.47
1:L:251:ARG:NH1	1:M:285:TYR:OH	2.47	0.47
3:R:6017:ILE:CG1	3:R:6188:LYS:HB2	2.44	0.47
3:R:6116:THR:HG21	3:R:6147:ILE:CD1	2.44	0.47
3:P:7007:THR:O	3:P:7011:LEU:HD13	2.14	0.47
1:O:81:ILE:HG22	4:S:14:DG:P	2.53	0.47
1:O:246:ASP:N	1:O:246:ASP:OD1	2.46	0.47
3:Q:5064:LEU:HD21	3:Q:5083:ILE:HD13	1.95	0.47
3:R:6034:VAL:HG13	3:R:6101:VAL:HG21	1.96	0.47
1:B:290:GLU:HG2	1:B:294:TYR:HE2	1.79	0.47
3:F:7039:TYR:C	3:F:7039:TYR:CD1	2.87	0.47
3:Q:5182:ILE:HD13	3:Q:5218:VAL:HG21	1.96	0.47
1:O:213:SER:CA	2:K:148:ASN:ND2	2.73	0.47
3:R:6032:ARG:HB3	3:R:6039:TYR:HD1	1.78	0.47
1:C:97:PHE:CB	3:G:5205:GLY:O	2.60	0.47
2:A:114:LEU:HD23	2:A:114:LEU:HA	1.75	0.47
1:O:48:HIS:CE1	1:O:141:ILE:HD11	2.49	0.47
1:B:44:HIS:HE1	1:B:133:SER:HA	1.79	0.47
1:N:165:LYS:HG2	1:N:169:MET:HE3	1.96	0.47
2:A:130:ARG:HD2	2:A:130:ARG:O	2.14	0.47
1:E:290:GLU:HG2	1:E:294:TYR:HE2	1.79	0.47
1:L:57:THR:HG23	6:L:700:08T:O1B	2.13	0.47
2:K:102:VAL:O	2:K:102:VAL:HG22	2.14	0.47
3:P:7010:LEU:O	3:P:7014:PHE:CD1	2.67	0.47
1:O:81:ILE:HG22	4:S:14:DG:OP1	2.14	0.47
3:R:6180:PHE:HD1	3:R:6220:LEU:HD22	1.79	0.47
3:R:6023:LEU:HD13	3:R:6048:ILE:HG21	1.95	0.47
5:T:5:DA:OP2	5:T:5:DA:H2'	2.14	0.47
4:I:9:DT:H2'	4:I:9:DT:O2	2.15	0.47
3:P:7137:THR:HG22	3:P:7138:ILE:N	2.29	0.47
1:D:3:THR:CG2	1:D:18:SER:HB2	2.44	0.47
1:L:186:ALA:HB3	1:L:219:VAL:HG22	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:307:TYR:CD1	1:C:289:GLY:HA3	2.49	0.47
2:A:85:ILE:O	2:A:85:ILE:CG2	2.62	0.47
1:C:297:ILE:HG23	1:D:297:ILE:HG13	1.96	0.47
1:O:251:ARG:CD	2:K:71:GLN:HA	2.44	0.47
1:N:83:PHE:O	1:N:87:PRO:HD2	2.14	0.47
1:N:185:ILE:HD13	1:N:215:SER:CB	2.44	0.47
3:G:5004:SER:N	3:G:5046:ASP:OD2	2.40	0.47
1:L:260:ASP:OD1	1:L:260:ASP:O	2.33	0.47
2:K:76:MET:HE1	2:K:79:VAL:HB	1.97	0.47
1:C:48:HIS:CE1	1:C:141:ILE:CD1	2.84	0.47
1:N:49:SER:OG	1:N:50:PRO:HA	2.14	0.47
3:G:5052:VAL:CG2	3:G:5053:ALA:N	2.77	0.47
3:H:6152:PHE:CD2	3:H:6163:VAL:HA	2.50	0.47
3:P:7135:ILE:HG23	3:P:7152:PHE:N	2.30	0.47
1:M:119:ARG:O	1:M:122:ARG:HG2	2.15	0.47
3:F:7010:LEU:O	3:F:7014:PHE:HD1	1.98	0.47
1:N:42:ILE:N	1:N:101:GLN:HE21	2.10	0.47
1:N:42:ILE:HG22	1:N:43:PRO:O	2.15	0.47
3:R:6087:ARG:HH11	3:R:6087:ARG:HG3	1.79	0.47
1:N:213:SER:HB3	1:O:153:ARG:NH1	2.28	0.47
1:M:29:ASP:HA	1:M:32:THR:CG2	2.44	0.47
1:M:3:THR:HG1	1:M:22:GLU:CD	2.18	0.47
1:M:251:ARG:NH1	1:M:251:ARG:CG	2.78	0.47
3:P:7001:MSE:N	3:P:7072:GLU:CG	2.78	0.47
1:D:38:SER:C	1:D:40:GLY:N	2.66	0.47
3:P:7176:ASN:HB2	3:P:7227:ASP:HB3	1.96	0.47
1:C:176:LEU:HD22	1:C:211:LEU:HD22	1.97	0.47
1:L:34:LYS:HB3	1:L:34:LYS:HE3	1.56	0.47
1:O:273:TYR:CD1	1:O:281:ILE:HD13	2.49	0.47
2:A:85:ILE:HG22	2:A:89:LEU:CD1	2.43	0.47
1:E:307:TYR:CD2	2:A:80:TYR:CD1	3.02	0.47
2:K:167:LEU:CD1	2:K:180:LEU:HG	2.45	0.47
1:E:277:THR:CG2	1:E:317:GLN:O	2.49	0.47
1:B:48:HIS:NE2	1:B:141:ILE:HD11	2.29	0.47
1:O:209:GLY:O	2:K:144:ILE:HD13	2.14	0.47
1:C:204:PHE:HB2	6:C:700:08T:C8	2.44	0.47
6:C:700:08T:C2'	6:C:700:08T:N3	2.72	0.47
1:O:14:LYS:O	1:O:14:LYS:HG3	2.15	0.47
1:E:10:ILE:HD13	2:A:141:TYR:HD2	1.75	0.47
1:C:246:ASP:N	1:C:246:ASP:OD1	2.48	0.47
3:G:5076:SER:O	3:G:5077:GLU:C	2.53	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:7021:ILE:CG1	3:P:7022:MSE:N	2.78	0.47
3:R:6011:LEU:HD22	3:R:6057:LEU:HD11	1.95	0.47
3:R:6150:ASN:HA	3:R:6165:TYR:O	2.15	0.47
3:R:6138:ILE:CG1	3:R:6184:MSE:HE3	2.44	0.47
1:D:42:ILE:HG22	1:D:43:PRO:O	2.15	0.47
2:A:124:ILE:HD13	2:A:139:ILE:HD11	1.97	0.47
1:O:282:ILE:O	1:O:286:GLU:HG3	2.13	0.47
1:M:290:GLU:HG2	1:M:294:TYR:HE2	1.80	0.47
3:Q:5189:MSE:HB3	3:Q:5216:TYR:CD2	2.50	0.47
3:G:5142:VAL:HG21	3:G:5172:TYR:CD2	2.50	0.47
3:H:6067:VAL:HG12	3:H:6071:ALA:HB2	1.96	0.47
1:E:121:LEU:O	1:E:125:MET:HG3	2.14	0.47
1:L:20:ILE:HD13	1:L:63:LEU:HD23	1.96	0.47
1:E:51:SER:O	1:E:54:THR:HG23	2.15	0.47
3:Q:5067:VAL:HB	3:Q:5085:ASP:OD2	2.14	0.47
3:R:6096:ASP:OD1	3:R:6097:PRO:HD2	2.15	0.47
1:L:200:ASN:HD21	1:L:210:GLU:HG3	1.79	0.47
1:E:114:LEU:HD13	1:E:114:LEU:H	1.80	0.47
1:D:84:VAL:HA	1:D:88:LEU:HB2	1.97	0.47
2:K:152:PRO:HD2	2:K:153:LEU:H	1.79	0.47
3:G:5092:TRP:CD1	3:G:5093:PRO:CD	2.98	0.47
1:C:71:MET:HE1	1:C:73:PHE:HD1	1.78	0.47
3:R:6019:SER:OG	3:R:6020:GLY:N	2.45	0.47
1:M:247:VAL:O	1:M:248:LYS:C	2.54	0.47
5:T:13:DA:H2"	5:T:14:DG:OP2	2.15	0.47
1:B:271:GLU:O	1:B:275:ARG:HD2	2.15	0.47
2:A:78:ALA:CB	2:A:101:ALA:HB1	2.44	0.47
1:D:235:ILE:O	1:D:235:ILE:HG22	2.14	0.47
1:L:12:GLU:HA	1:L:208:ILE:HG21	1.97	0.47
1:L:307:TYR:HE1	1:M:286:GLU:HA	1.80	0.47
1:N:256:LYS:NZ	1:O:159:GLN:HE22	2.13	0.47
1:M:53:GLY:O	6:M:700:08T:H14	2.15	0.47
1:M:57:THR:OG1	6:M:700:08T:O1B	2.14	0.47
1:O:303:LEU:CD1	2:K:70:SER:HB2	2.45	0.47
1:C:232:ARG:NE	1:C:260:ASP:OD2	2.48	0.47
1:M:276:VAL:HG22	1:M:277:THR:N	2.29	0.47
1:E:61:LYS:CG	1:E:71:MET:HE1	2.38	0.47
2:A:137:ASP:O	2:A:141:TYR:HD1	1.98	0.47
3:G:5116:THR:HG21	3:G:5169:LEU:HD13	1.97	0.47
2:A:109:GLY:HA2	4:I:8:DT:C1'	2.44	0.47
3:P:7154:LYS:HG3	3:P:7160:LEU:HD21	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:49:SER:OG	1:B:50:PRO:HA	2.15	0.47
1:D:242:LEU:CD1	1:D:250:LEU:HD21	2.45	0.47
1:D:191:LYS:CD	1:M:186:ALA:HB2	2.45	0.47
3:P:7082:LYS:HE2	3:P:7084:ALA:HB2	1.97	0.47
1:L:72:MET:HE2	3:Q:5156:GLU:HA	1.97	0.47
1:B:96:SER:HB3	1:B:102:LYS:HE2	1.97	0.47
1:E:204:PHE:O	1:E:207:THR:HG22	2.14	0.47
1:B:34:LYS:HE3	1:B:34:LYS:HB3	1.53	0.47
1:N:276:VAL:CG2	1:N:318:TRP:HB3	2.36	0.47
2:K:6:ASP:OD1	2:K:6:ASP:O	2.33	0.47
1:N:251:ARG:CG	1:N:251:ARG:NH1	2.78	0.47
3:P:7146:LYS:HA	3:P:7171:ASP:HA	1.96	0.47
3:P:7022:MSE:HE3	3:P:7023:LEU:C	2.35	0.47
1:C:276:VAL:HG22	1:C:277:THR:N	2.30	0.47
1:M:201:PHE:HB3	1:M:202:PRO:HD3	1.97	0.47
2:K:63:PHE:O	2:K:67:ASN:HB2	2.15	0.47
1:M:5:ASN:C	1:M:7:LYS:H	2.18	0.47
2:K:47:ILE:HG21	2:K:98:LEU:HB3	1.96	0.46
3:R:6027:GLN:HE21	3:R:6047:VAL:HB	1.79	0.46
3:R:6032:ARG:HB2	3:R:6038:THR:O	2.15	0.46
3:G:5200:ALA:HB1	3:G:5226:HIS:CD2	2.49	0.46
1:C:5:ASN:C	1:C:7:LYS:H	2.17	0.46
1:D:247:VAL:O	1:D:248:LYS:C	2.53	0.46
1:N:55:GLY:O	1:N:59:VAL:HG23	2.14	0.46
1:D:276:VAL:HG23	1:D:318:TRP:CB	2.24	0.46
2:A:3:LEU:O	2:A:4:PHE:HB2	2.15	0.46
1:D:251:ARG:HH11	1:D:251:ARG:CG	2.27	0.46
3:H:6030:MSE:HG3	3:H:6103:PRO:CG	2.38	0.46
3:H:6032:ARG:HB3	3:H:6103:PRO:HB3	1.96	0.46
3:G:5190:GLN:HG2	3:G:5216:TYR:OH	2.14	0.46
1:B:242:LEU:CD1	1:B:250:LEU:HD21	2.44	0.46
1:N:29:ASP:CA	1:N:32:THR:HG22	2.44	0.46
1:D:213:SER:HB3	1:E:153:ARG:HD2	1.96	0.46
1:L:232:ARG:CG	1:L:233:GLY:N	2.78	0.46
5:J:19:DT:H1'	5:J:20:DA:H5'	1.97	0.46
1:L:290:GLU:HG2	1:L:294:TYR:HE2	1.81	0.46
1:D:83:PHE:O	1:D:87:PRO:HD2	2.14	0.46
1:M:16:ARG:O	1:M:16:ARG:HG2	2.15	0.46
3:P:7045:SER:HB2	3:P:7046:ASP:OD1	2.15	0.46
1:N:238:VAL:O	1:N:242:LEU:HD13	2.15	0.46
3:P:7219:ALA:O	3:P:7220:LEU:HD23	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:57:THR:HG23	1:N:137:THR:HG21	1.95	0.46
3:H:6080:ASN:HA	3:H:6094:ALA:CB	2.45	0.46
3:G:5037:THR:HG21	3:G:5186:ASN:CG	2.36	0.46
1:O:276:VAL:HA	1:O:318:TRP:CB	2.46	0.46
1:C:80:LYS:HB3	4:I:18:DT:OP2	2.15	0.46
1:D:5:ASN:C	1:D:7:LYS:H	2.18	0.46
1:L:200:ASN:OD1	1:L:200:ASN:N	2.49	0.46
1:N:247:VAL:O	1:N:248:LYS:C	2.53	0.46
3:P:7126:LEU:O	3:P:7126:LEU:HD12	2.16	0.46
1:C:297:ILE:HG21	1:D:297:ILE:HG13	1.96	0.46
1:D:81:ILE:HD11	1:D:120:HIS:HB2	1.96	0.46
3:P:7007:THR:HG23	3:P:7044:ILE:CG1	2.33	0.46
2:K:3:LEU:HB2	2:K:4:PHE:CD2	2.51	0.46
1:E:251:ARG:NH1	1:E:251:ARG:CG	2.75	0.46
1:L:239:LEU:O	1:L:243:LYS:HG3	2.14	0.46
1:B:246:ASP:OD1	1:B:246:ASP:N	2.44	0.46
1:B:145:ILE:HD11	1:B:148:LEU:HD12	1.96	0.46
2:K:150:LYS:C	2:K:152:PRO:CD	2.81	0.46
2:K:154:VAL:O	2:K:158:LEU:HG	2.16	0.46
3:F:7044:ILE:HD12	3:F:7044:ILE:H	1.81	0.46
3:P:7130:SER:O	3:P:7134:GLN:N	2.49	0.46
3:R:6066:LEU:HD12	3:R:6067:VAL:HG23	1.97	0.46
1:B:238:VAL:HG22	1:B:253:LEU:HD13	1.96	0.46
3:Q:5154:LYS:HG3	3:Q:5154:LYS:O	2.16	0.46
3:H:6076:SER:HB2	3:H:6082:LYS:HB2	1.95	0.46
1:E:23:CYS:HB2	1:E:25:LEU:HD11	1.97	0.46
3:H:6154:LYS:HG3	3:H:6154:LYS:O	2.16	0.46
1:C:235:ILE:HG22	1:C:235:ILE:O	2.15	0.46
4:S:25:DG:H2"	4:S:26:DT:OP2	2.15	0.46
3:P:7149:ILE:O	3:P:7166:SER:HA	2.14	0.46
1:D:42:ILE:N	1:D:101:GLN:HE21	2.11	0.46
1:B:56:LYS:N	6:B:700:08T:O2B	2.48	0.46
1:B:15:TYR:CZ	1:B:179:ILE:HG23	2.51	0.46
1:N:282:ILE:O	1:N:286:GLU:HG3	2.15	0.46
1:L:5:ASN:C	1:L:7:LYS:H	2.18	0.46
1:E:24:ILE:HG22	1:E:168:MET:HG2	1.96	0.46
1:M:96:SER:HB2	1:M:102:LYS:HE2	1.98	0.46
1:M:5:ASN:O	1:M:7:LYS:N	2.48	0.46
1:L:297:ILE:HG22	1:M:295:HIS:O	2.15	0.46
1:B:88:LEU:HD12	1:B:88:LEU:HA	1.73	0.46
1:E:235:ILE:HG22	1:E:235:ILE:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:122:ARG:HH11	1:N:122:ARG:HG2	1.80	0.46
1:E:276:VAL:HG22	1:E:277:THR:N	2.31	0.46
1:O:14:LYS:HG2	1:O:15:TYR:CE1	2.51	0.46
1:B:303:LEU:HD22	1:C:265:VAL:HG11	1.93	0.46
1:N:227:LEU:O	1:N:230:ASN:HB3	2.15	0.46
1:C:32:THR:O	1:C:36:ILE:HG13	2.15	0.46
3:H:6010:LEU:O	3:H:6013:ASN:N	2.45	0.46
1:E:3:THR:OG1	1:E:18:SER:HB2	2.15	0.46
2:K:22:TRP:HA	2:K:25:VAL:HB	1.97	0.46
4:I:12:DA:H8	4:I:12:DA:OP2	1.99	0.46
3:R:6187:MSE:HE3	3:R:6187:MSE:HB3	1.53	0.46
1:O:114:LEU:HD13	1:O:114:LEU:H	1.81	0.46
1:D:276:VAL:HG22	1:D:277:THR:N	2.31	0.46
4:I:16:DA:C2	4:I:17:DC:C4	3.04	0.46
1:C:251:ARG:NH1	1:C:251:ARG:CG	2.75	0.46
2:A:47:ILE:HG21	2:A:98:LEU:HB3	1.97	0.46
1:B:81:ILE:HG23	1:B:82:ASP:N	2.29	0.46
3:G:5143:LYS:HG3	3:G:5144:GLU:HG3	1.96	0.46
3:G:5201:LYS:O	3:G:5204:GLN:HB2	2.15	0.46
3:H:6021:ILE:HG22	3:H:6057:LEU:HD13	1.98	0.46
1:O:10:ILE:HD13	2:K:141:TYR:CE2	2.50	0.46
3:H:6127:LEU:O	3:H:6130:SER:HB3	2.15	0.46
3:G:5195:LYS:HE3	3:G:5195:LYS:HB2	1.69	0.46
1:D:151:ARG:HG3	1:D:151:ARG:HH11	1.81	0.46
1:N:297:ILE:HG23	1:O:297:ILE:HG13	1.98	0.46
1:B:81:ILE:HD13	1:B:116:GLU:HG3	1.98	0.46
1:C:49:SER:OG	1:C:50:PRO:HA	2.15	0.46
1:C:49:SER:N	1:C:56:LYS:HD3	2.30	0.46
2:A:109:GLY:CA	4:I:8:DT:C1'	2.94	0.46
1:M:214:TYR:O	1:M:224:ILE:HD13	2.16	0.46
3:G:5056:ASP:HB3	3:G:5092:TRP:HZ2	1.79	0.46
3:R:6113:SER:HB3	3:R:6228:PHE:CE2	2.51	0.46
3:Q:5060:PHE:HD1	3:Q:5092:TRP:CD2	2.33	0.46
3:F:7203:LYS:HA	3:F:7203:LYS:HD3	1.54	0.46
1:O:175:ARG:O	1:O:179:ILE:HG13	2.16	0.46
4:I:25:DG:H2"	4:I:26:DT:C6	2.51	0.46
3:P:7021:ILE:CG1	3:P:7022:MSE:H	2.28	0.46
1:E:242:LEU:CD1	1:E:250:LEU:HD21	2.45	0.46
4:S:22:DA:C2	5:T:10:DA:C2	3.03	0.46
1:B:282:ILE:O	1:B:286:GLU:HG3	2.15	0.46
2:A:165:ASP:O	2:A:168:LYS:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:254:ALA:N	1:N:255:PRO:HD2	2.31	0.46
1:E:294:TYR:HB3	2:A:84:LEU:HD22	1.98	0.46
2:A:55:ILE:CG1	2:A:56:ALA:N	2.69	0.46
1:C:299:ALA:CB	1:D:295:HIS:HD2	2.15	0.46
1:C:108:GLU:HG3	1:D:122:ARG:HG3	1.98	0.46
1:N:303:LEU:HD21	1:O:288:VAL:HG12	1.98	0.46
1:L:81:ILE:HG23	1:L:82:ASP:N	2.31	0.46
3:R:6073:ILE:HG23	3:R:6083:ILE:HG12	1.98	0.46
1:L:285:TYR:HD2	2:K:97:TYR:CB	2.28	0.46
1:B:16:ARG:NH2	6:B:700:08T:H2	2.30	0.46
1:M:80:LYS:NZ	4:S:17:DC:P	2.89	0.46
1:B:30:LYS:O	1:B:34:LYS:HG2	2.15	0.46
1:L:225:LEU:HD12	1:L:229:THR:HG23	1.98	0.46
1:D:15:TYR:O	1:D:17:PRO:HD3	2.15	0.46
3:P:7203:LYS:HE3	3:P:7203:LYS:HB2	1.77	0.46
1:D:271:GLU:O	1:D:275:ARG:HD2	2.16	0.45
1:M:108:GLU:OE2	6:M:700:08T:F1	2.24	0.45
1:C:77:SER:HA	1:C:114:LEU:HD11	1.98	0.45
1:L:276:VAL:HG22	1:L:277:THR:N	2.30	0.45
4:I:28:DT:H2"	4:I:29:DG:OP2	2.16	0.45
3:R:6115:VAL:CG1	3:R:6197:LEU:HD23	2.40	0.45
3:G:5226:HIS:HD2	3:G:5228:PHE:HB2	1.76	0.45
2:A:122:LEU:HD22	2:A:126:LEU:HD11	1.96	0.45
1:M:224:ILE:O	1:M:228:VAL:HG23	2.16	0.45
1:C:17:PRO:HB3	1:C:22:GLU:HB3	1.97	0.45
3:H:6104:ASN:CG	3:H:6104:ASN:O	2.55	0.45
1:D:49:SER:N	1:D:56:LYS:HD3	2.31	0.45
2:K:151:LEU:N	2:K:152:PRO:CD	2.79	0.45
3:H:6157:ASP:C	3:H:6159:ALA:H	2.18	0.45
3:P:7052:VAL:HG21	3:P:7081:ILE:HD11	1.99	0.45
5:J:7:DA:H2"	5:J:8:DC:O5'	2.16	0.45
3:F:7014:PHE:CE1	3:F:7029:ILE:HD11	2.51	0.45
1:O:242:LEU:HD12	1:O:250:LEU:HD11	1.98	0.45
3:R:6092:TRP:CD1	3:R:6093:PRO:HD2	2.51	0.45
1:B:225:LEU:HD12	1:B:229:THR:HG23	1.98	0.45
1:D:68:ASN:O	1:D:100:ARG:HD3	2.16	0.45
1:O:235:ILE:HG22	1:O:235:ILE:O	2.16	0.45
2:K:98:LEU:O	2:K:102:VAL:HG12	2.17	0.45
1:E:251:ARG:NE	2:A:71:GLN:OE1	2.44	0.45
4:S:25:DG:H5'	4:S:25:DG:C8	2.50	0.45
3:R:6003:LEU:HD22	3:R:6007:THR:CG2	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:137:ASP:O	2:K:141:TYR:HD1	1.99	0.45
1:L:192:VAL:CG1	1:L:220:LEU:HD23	2.47	0.45
1:B:251:ARG:CG	1:B:251:ARG:NH1	2.80	0.45
1:M:154:VAL:HG12	1:M:154:VAL:O	2.15	0.45
3:P:7126:LEU:C	3:P:7126:LEU:HD12	2.37	0.45
3:Q:5096:ASP:OD1	3:Q:5097:PRO:HD2	2.16	0.45
1:L:96:SER:HB3	1:L:102:LYS:HE2	1.97	0.45
3:F:7163:VAL:O	3:F:7163:VAL:HG13	2.16	0.45
3:F:7151:GLY:N	3:F:7165:TYR:O	2.44	0.45
1:O:81:ILE:HG13	1:O:85:ARG:NH1	2.31	0.45
1:L:125:MET:O	1:L:129:SER:HB2	2.17	0.45
3:H:6021:ILE:HG12	3:H:6022:MSE:N	2.32	0.45
3:R:6002:LYS:HG2	3:R:6070:ASP:O	2.16	0.45
1:M:175:ARG:HG3	1:M:175:ARG:NH1	2.26	0.45
2:A:62:LYS:HE3	2:A:91:ASP:OD1	2.17	0.45
1:E:141:ILE:C	1:E:143:GLY:N	2.69	0.45
2:K:78:ALA:CB	2:K:101:ALA:HB1	2.46	0.45
3:P:7150:ASN:HB3	3:P:7163:VAL:CG2	2.46	0.45
1:D:95:ALA:HB2	3:G:5096:ASP:HA	1.96	0.45
3:R:6023:LEU:HD12	3:R:6023:LEU:C	2.36	0.45
2:K:149:GLY:C	2:K:151:LEU:N	2.70	0.45
3:F:7014:PHE:CD2	3:F:7031:THR:HG22	2.43	0.45
5:T:11:DC:H2"	5:T:12:DG:C8	2.51	0.45
2:A:61:SER:O	2:A:65:VAL:HG23	2.17	0.45
1:B:98:ASP:HB2	1:B:100:ARG:HG3	1.98	0.45
1:L:251:ARG:HD2	1:M:285:TYR:OH	2.16	0.45
3:Q:5055:TYR:HB2	3:Q:5095:ALA:CB	2.46	0.45
1:L:232:ARG:CG	1:L:233:GLY:H	2.28	0.45
2:A:121:VAL:HG12	2:A:170:VAL:HG13	1.98	0.45
1:N:8:GLU:OE2	1:N:13:GLN:HB3	2.17	0.45
1:N:260:ASP:O	1:N:260:ASP:OD1	2.34	0.45
4:I:11:DT:H71	4:I:11:DT:OP2	2.16	0.45
3:F:7003:LEU:HA	3:F:7003:LEU:HD23	1.62	0.45
1:M:77:SER:OG	1:N:120:HIS:HA	2.16	0.45
1:N:110:ASP:HB3	1:N:138:ALA:HB1	1.98	0.45
1:B:48:HIS:HA	1:B:138:ALA:O	2.17	0.45
1:L:121:LEU:O	1:L:125:MET:HG3	2.16	0.45
3:H:6018:ASN:HB3	3:H:6031:THR:HG21	1.97	0.45
3:R:6087:ARG:HG3	3:R:6087:ARG:NH1	2.31	0.45
1:D:224:ILE:O	1:D:228:VAL:HG23	2.16	0.45
3:R:6176:ASN:CG	3:R:6228:PHE:CE1	2.89	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:288:VAL:HG22	1:M:308:LEU:HD11	1.98	0.45
3:F:7121:GLU:HG2	3:F:7121:GLU:O	2.16	0.45
1:O:260:ASP:O	1:O:260:ASP:OD1	2.34	0.45
1:C:291:ASN:ND2	1:C:304:HIS:CE1	2.84	0.45
3:Q:5078:ASP:C	3:Q:5080:ASN:N	2.69	0.45
1:O:11:LEU:HG	1:O:212:ASP:CG	2.37	0.45
1:C:110:ASP:HB3	1:C:138:ALA:HB1	1.99	0.45
2:A:120:GLU:HG3	2:A:142:LYS:HZ1	1.81	0.45
1:N:38:SER:O	1:N:40:GLY:N	2.50	0.45
1:D:220:LEU:HA	1:D:224:ILE:HD12	1.97	0.45
5:T:8:DC:C2	5:T:9:DT:C4	3.04	0.45
1:O:121:LEU:O	1:O:125:MET:HG3	2.17	0.45
3:F:7008:THR:HG22	3:F:7064:LEU:HD23	1.99	0.45
1:C:85:ARG:O	1:C:89:THR:HB	2.16	0.45
1:N:48:HIS:CE1	1:N:141:ILE:CD1	2.87	0.45
3:G:5209:PHE:HB2	3:G:5216:TYR:HB2	1.98	0.45
3:P:7113:SER:HB3	3:P:7228:PHE:CE2	2.52	0.45
3:F:7208:LYS:HE3	3:F:7215:ASN:HB3	1.98	0.45
3:R:6130:SER:OG	3:R:6135:ILE:HB	2.17	0.45
6:B:700:08T:O2'	6:B:700:08T:N3	2.46	0.45
2:K:162:VAL:O	2:K:162:VAL:CG1	2.63	0.45
5:T:8:DC:H2"	5:T:9:DT:C7	2.47	0.45
5:T:8:DC:C2'	5:T:9:DT:H72	2.46	0.45
1:O:291:ASN:ND2	1:O:304:HIS:CE1	2.85	0.45
1:E:165:LYS:HG3	1:E:201:PHE:CE2	2.52	0.45
1:D:206:LYS:O	1:D:210:GLU:HG2	2.16	0.45
1:N:17:PRO:HB3	1:N:22:GLU:HB3	1.98	0.45
3:H:6116:THR:HB	3:H:6147:ILE:HD12	1.97	0.45
2:K:121:VAL:HG12	2:K:170:VAL:HG13	1.98	0.45
1:O:109:PHE:CE2	1:O:118:GLN:HG2	2.52	0.45
1:E:243:LYS:CA	1:E:318:TRP:HZ2	2.29	0.45
3:F:7102:ALA:HB1	3:F:7103:PRO:CD	2.46	0.45
1:B:81:ILE:CG2	1:B:82:ASP:N	2.80	0.45
1:M:84:VAL:HA	1:M:88:LEU:HB2	1.98	0.45
3:F:7226:HIS:CG	3:F:7227:ASP:H	2.35	0.45
1:D:47:LEU:HD22	1:D:157:PHE:CE1	2.50	0.45
1:D:191:LYS:HD3	1:M:186:ALA:HA	1.97	0.45
1:C:29:ASP:O	1:C:32:THR:HG22	2.17	0.45
1:C:75:ASN:HB3	1:C:78:ASP:HB2	1.98	0.45
1:L:254:ALA:N	1:L:255:PRO:HD2	2.32	0.45
1:O:271:GLU:O	1:O:275:ARG:HD2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:85:ILE:O	2:A:85:ILE:HG22	2.17	0.45
1:M:141:ILE:O	1:M:143:GLY:N	2.50	0.45
1:N:245:LYS:NZ	1:N:317:GLN:HE21	2.15	0.45
3:R:6055:TYR:HB2	3:R:6095:ALA:CB	2.47	0.45
1:E:14:LYS:O	1:E:14:LYS:HG3	2.16	0.45
1:M:32:THR:O	1:M:36:ILE:HG13	2.17	0.45
1:N:230:ASN:ND2	1:N:231:ASP:OD1	2.50	0.45
1:L:232:ARG:HH11	1:L:233:GLY:N	2.13	0.45
3:H:6027:GLN:HG3	3:H:6047:VAL:HG22	1.99	0.45
1:E:260:ASP:O	1:E:260:ASP:OD1	2.34	0.45
1:M:235:ILE:O	1:M:235:ILE:HG22	2.17	0.45
1:B:293:GLN:CD	2:A:84:LEU:O	2.49	0.44
1:N:243:LYS:CG	1:N:318:TRP:CZ2	3.00	0.44
2:K:4:PHE:CE2	3:P:7032:ARG:HD2	2.52	0.44
1:E:214:TYR:O	1:E:217:LYS:HG2	2.17	0.44
1:N:56:LYS:N	6:N:700:08T:O2B	2.50	0.44
5:J:4:DG:H1'	5:J:5:DA:O5'	2.16	0.44
3:G:5200:ALA:HB1	3:G:5226:HIS:NE2	2.32	0.44
1:B:15:TYR:O	1:B:17:PRO:HD3	2.17	0.44
1:L:251:ARG:NH1	1:L:251:ARG:CG	2.80	0.44
1:B:162:ASP:O	1:B:166:ILE:HG13	2.17	0.44
1:B:67:VAL:HG12	1:B:67:VAL:O	2.18	0.44
1:C:151:ARG:HG3	1:C:151:ARG:HH11	1.81	0.44
2:A:55:ILE:C	2:A:57:GLN:N	2.69	0.44
1:N:276:VAL:HG22	1:N:277:THR:N	2.32	0.44
2:A:75:CYS:C	2:A:77:PRO:HD2	2.38	0.44
1:C:88:LEU:HD23	1:C:88:LEU:HA	1.80	0.44
1:E:246:ASP:OD1	1:E:246:ASP:N	2.44	0.44
6:B:700:08T:F1	6:B:700:08T:O1B	2.25	0.44
1:O:242:LEU:CD1	1:O:250:LEU:HD21	2.46	0.44
1:B:71:MET:HE3	1:B:105:VAL:HG21	1.99	0.44
1:C:64:CYS:HB3	1:C:69:ALA:HB3	1.99	0.44
1:M:90:ASN:HB3	3:Q:5035:ASN:ND2	2.32	0.44
1:D:297:ILE:CG2	1:E:293:GLN:O	2.66	0.44
3:Q:5076:SER:O	3:Q:5078:ASP:O	2.36	0.44
1:D:110:ASP:HB3	1:D:138:ALA:HB1	1.99	0.44
1:D:95:ALA:H	3:G:5095:ALA:HA	1.81	0.44
3:R:6081:ILE:HG22	3:R:6082:LYS:N	2.32	0.44
1:B:49:SER:HB3	1:B:56:LYS:HZ2	1.83	0.44
1:N:213:SER:CB	1:O:153:ARG:CZ	2.93	0.44
1:C:94:ALA:O	1:C:102:LYS:HE3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:105:GLY:O	2:A:106:LYS:HE2	2.18	0.44
2:A:72:PHE:N	2:A:72:PHE:CD1	2.85	0.44
3:P:7188:LYS:HA	3:P:7188:LYS:HD3	1.85	0.44
3:R:6133:LEU:O	3:R:6133:LEU:HG	2.17	0.44
3:Q:5227:ASP:O	3:Q:5227:ASP:OD1	2.35	0.44
1:O:294:TYR:HB3	2:K:84:LEU:HD22	1.99	0.44
2:K:55:ILE:C	2:K:57:GLN:N	2.70	0.44
3:P:7028:PHE:HE2	3:P:7030:MSE:CE	2.26	0.44
3:F:7115:VAL:HG13	3:F:7197:LEU:HD23	1.99	0.44
3:P:7153:ASN:O	3:P:7157:ASP:N	2.50	0.44
3:P:7182:ILE:HG22	3:P:7183:ASN:O	2.16	0.44
1:O:183:GLU:HB3	1:O:185:ILE:HG13	1.99	0.44
2:A:155:LEU:HD22	2:A:183:LEU:CD2	2.34	0.44
1:D:49:SER:OG	1:D:50:PRO:HA	2.17	0.44
3:R:6149:ILE:O	3:R:6166:SER:HA	2.18	0.44
3:P:7130:SER:HB3	3:P:7135:ILE:O	2.17	0.44
1:B:292:ASN:HD22	2:A:88:GLY:HA3	1.82	0.44
1:E:15:TYR:CE2	1:E:179:ILE:HG23	2.53	0.44
1:D:165:LYS:HG2	1:D:169:MET:HE2	2.00	0.44
3:P:7180:PHE:CD2	3:P:7198:LEU:HD13	2.52	0.44
3:H:6189:MSE:HE3	3:H:6189:MSE:HB3	1.85	0.44
3:F:7055:TYR:HB2	3:F:7095:ALA:HB2	1.99	0.44
1:N:67:VAL:CG1	1:N:67:VAL:O	2.65	0.44
1:L:232:ARG:NH1	1:L:233:GLY:H	2.14	0.44
3:F:7015:ALA:HA	3:F:7057:LEU:HD23	2.00	0.44
1:M:81:ILE:HD11	1:M:120:HIS:HB2	1.99	0.44
1:N:81:ILE:HD11	1:N:120:HIS:HB2	2.00	0.44
3:H:6090:ILE:HG12	3:F:7165:TYR:HD1	1.81	0.44
1:N:49:SER:N	1:N:56:LYS:HD3	2.33	0.44
1:L:246:ASP:OD1	1:L:246:ASP:N	2.51	0.44
2:A:150:LYS:C	2:A:152:PRO:CD	2.82	0.44
1:B:272:ILE:O	1:B:276:VAL:HG12	2.18	0.44
4:I:14:DG:N2	5:J:17:DC:C2	2.82	0.44
3:H:6194:TYR:OH	3:H:6216:TYR:HE2	2.01	0.44
1:B:251:ARG:NH2	1:C:270:GLU:HA	2.33	0.44
1:L:288:VAL:HG22	1:L:308:LEU:HD11	2.00	0.44
3:H:6105:LYS:HA	3:H:6106:PRO:HD3	1.81	0.44
3:G:5062:GLY:O	3:G:5065:SER:OG	2.30	0.44
1:M:297:ILE:HG23	1:N:297:ILE:HG13	1.98	0.44
2:K:75:CYS:C	2:K:77:PRO:HD2	2.37	0.44
1:D:141:ILE:O	1:D:143:GLY:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:12:GLU:HG3	1:E:13:GLN:N	2.31	0.44
1:C:243:LYS:HG2	1:C:318:TRP:NE1	2.32	0.44
1:B:250:LEU:HD23	1:B:250:LEU:HA	1.79	0.44
3:F:7189:MSE:CE	3:F:7209:PHE:CD1	3.01	0.44
1:L:44:HIS:HE1	1:L:133:SER:HA	1.83	0.44
1:O:277:THR:CG2	1:O:317:GLN:O	2.53	0.44
3:G:5113:SER:HB3	3:G:5228:PHE:CZ	2.53	0.44
3:P:7112:ALA:HB2	3:P:7197:LEU:HD22	2.00	0.44
1:D:29:ASP:CA	1:D:32:THR:HG22	2.48	0.44
3:Q:5092:TRP:CD1	3:Q:5093:PRO:O	2.71	0.44
3:Q:5025:SER:HA	3:Q:5048:ILE:O	2.18	0.44
1:M:38:SER:C	1:M:40:GLY:N	2.71	0.44
1:B:165:LYS:HG2	1:B:169:MET:CE	2.47	0.44
3:F:7028:PHE:CE2	3:F:7030:MSE:SE	3.21	0.44
1:D:251:ARG:HH22	1:E:270:GLU:HA	1.75	0.44
1:B:120:HIS:CE1	2:A:25:VAL:HG12	2.53	0.44
2:A:149:GLY:C	2:A:151:LEU:N	2.71	0.44
1:L:285:TYR:HB2	2:K:97:TYR:HD1	1.83	0.44
1:C:119:ARG:O	1:C:122:ARG:NH1	2.50	0.44
1:D:231:ASP:HB3	1:D:263:TRP:CZ2	2.53	0.44
3:F:7066:LEU:HA	3:F:7066:LEU:HD23	1.67	0.44
3:G:5165:TYR:CD1	3:F:7090:ILE:HG13	2.51	0.44
1:E:3:THR:CG2	1:E:18:SER:HB2	2.48	0.44
3:Q:5092:TRP:C	3:Q:5092:TRP:CD1	2.91	0.44
1:M:94:ALA:O	1:M:102:LYS:HE3	2.18	0.44
3:P:7118:ILE:CG1	3:P:7119:LYS:H	2.26	0.43
1:D:88:LEU:HA	1:D:88:LEU:HD23	1.79	0.43
3:R:6044:ILE:HD11	3:R:6048:ILE:HD11	1.99	0.43
1:B:276:VAL:HG22	1:B:277:THR:N	2.33	0.43
1:C:271:GLU:O	1:C:275:ARG:HD2	2.18	0.43
3:Q:5107:ILE:HG22	3:Q:5108:PRO:O	2.17	0.43
1:E:282:ILE:O	1:E:286:GLU:HG3	2.18	0.43
3:Q:5127:LEU:CD2	3:Q:5184:MSE:HE1	2.48	0.43
1:L:98:ASP:HB2	1:L:100:ARG:HG3	1.98	0.43
1:E:201:PHE:O	1:E:202:PRO:C	2.55	0.43
3:F:7085:ASP:CG	3:F:7086:ALA:N	2.71	0.43
3:H:6181:ILE:HD12	3:H:6223:ASP:HB3	2.00	0.43
1:B:140:ASN:OD1	1:B:142:ASP:HB2	2.18	0.43
1:M:246:ASP:N	1:M:246:ASP:OD1	2.49	0.43
5:T:3:DA:C2'	5:T:4:DG:OP2	2.67	0.43
3:R:6138:ILE:HG22	3:R:6151:GLY:HA2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:192:VAL:CG1	1:B:220:LEU:HD23	2.47	0.43
5:T:8:DC:C2	5:T:9:DT:C5	3.06	0.43
1:C:214:TYR:O	1:C:224:ILE:HD13	2.17	0.43
1:E:291:ASN:ND2	1:E:304:HIS:CE1	2.86	0.43
3:G:5195:LYS:HG2	3:G:5197:LEU:HD21	1.99	0.43
1:D:8:GLU:OE2	1:D:13:GLN:HB3	2.17	0.43
1:C:288:VAL:HG22	1:C:308:LEU:HD11	1.99	0.43
1:O:23:CYS:HB2	1:O:25:LEU:HD11	2.00	0.43
1:B:189:ASP:OD1	1:B:191:LYS:HE2	2.18	0.43
1:L:74:VAL:HG11	1:L:83:PHE:CE2	2.53	0.43
2:K:108:TYR:HB3	4:S:7:DT:C7	2.48	0.43
2:K:150:LYS:CB	2:K:152:PRO:HD3	2.47	0.43
1:C:317:GLN:C	1:C:318:TRP:HE3	2.22	0.43
3:Q:5136:ASP:OD2	3:Q:5154:LYS:N	2.52	0.43
1:O:250:LEU:HA	1:O:250:LEU:HD23	1.83	0.43
1:C:121:LEU:HD12	1:C:121:LEU:HA	1.86	0.43
1:O:59:VAL:O	1:O:63:LEU:HG	2.19	0.43
1:D:288:VAL:HG22	1:D:308:LEU:HD11	2.00	0.43
4:I:15:DT:H3	5:J:16:DA:N6	2.15	0.43
1:E:239:LEU:O	1:E:243:LYS:HG3	2.18	0.43
1:N:242:LEU:CD1	1:N:250:LEU:HD21	2.47	0.43
1:D:91:PHE:CE1	1:D:102:LYS:HD3	2.53	0.43
3:P:7105:LYS:HB2	3:P:7106:PRO:HD2	2.00	0.43
3:R:6038:THR:O	3:R:6038:THR:HG23	2.18	0.43
2:A:152:PRO:HD2	2:A:153:LEU:H	1.82	0.43
3:P:7022:MSE:HE2	3:P:7024:LYS:HE3	2.01	0.43
3:G:5201:LYS:HB3	3:G:5204:GLN:HB2	1.99	0.43
2:A:8:ILE:O	2:A:9:GLN:C	2.57	0.43
1:O:217:LYS:HG3	1:O:219:VAL:H	1.83	0.43
1:C:310:ILE:CG1	1:D:285:TYR:CD2	2.93	0.43
1:C:42:ILE:HG22	1:C:43:PRO:O	2.18	0.43
1:D:191:LYS:HD3	1:M:186:ALA:CA	2.49	0.43
4:S:24:DT:H2'	4:S:24:DT:H6	1.57	0.43
3:H:6120:ALA:HB2	3:H:6192:GLY:HA2	1.99	0.43
1:C:290:GLU:HG2	1:C:294:TYR:HE2	1.83	0.43
1:M:49:SER:HB3	1:M:56:LYS:HZ2	1.78	0.43
3:Q:5210:GLU:HG3	3:Q:5215:ASN:ND2	2.32	0.43
1:N:88:LEU:HD23	1:N:88:LEU:HA	1.76	0.43
1:E:251:ARG:HH12	2:A:70:SER:HG	1.58	0.43
3:R:6052:VAL:HG22	3:R:6053:ALA:N	2.33	0.43
1:B:190:MET:C	1:B:192:VAL:H	2.20	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:239:LEU:O	1:O:243:LYS:HG3	2.18	0.43
1:D:232:ARG:C	1:D:234:ALA:N	2.69	0.43
1:B:54:THR:HG22	1:B:202:PRO:O	2.19	0.43
3:Q:5068:ASN:HB2	3:Q:5070:ASP:OD1	2.18	0.43
1:B:74:VAL:HG11	1:B:83:PHE:CE2	2.54	0.43
1:E:20:ILE:HG21	1:E:34:LYS:HD2	2.01	0.43
1:D:58:THR:HG1	6:D:700:08T:PA	2.42	0.43
2:A:150:LYS:CB	2:A:152:PRO:HD3	2.47	0.43
3:R:6115:VAL:HG11	3:R:6195:LYS:HE2	2.01	0.43
3:G:5116:THR:HB	3:G:5147:ILE:HD12	2.01	0.43
1:D:310:ILE:CG1	1:E:285:TYR:HD2	2.27	0.43
1:E:14:LYS:HG2	1:E:15:TYR:CE1	2.54	0.43
3:G:5124:GLN:NE2	3:G:5191:PRO:HB3	2.34	0.43
1:L:192:VAL:HG12	1:L:193:VAL:N	2.34	0.43
1:B:232:ARG:NE	1:B:233:GLY:H	2.16	0.43
1:D:29:ASP:O	1:D:32:THR:HG22	2.18	0.43
1:M:71:MET:HG2	1:M:72:MET:N	2.34	0.43
3:R:6060:PHE:HD2	3:R:6092:TRP:CD1	2.36	0.43
3:Q:5135:ILE:HG22	3:Q:5135:ILE:O	2.17	0.43
1:L:185:ILE:HD13	1:L:215:SER:HB2	2.01	0.43
1:N:312:LEU:HD23	1:N:312:LEU:HA	1.89	0.43
2:A:98:LEU:O	2:A:102:VAL:HG12	2.19	0.43
2:A:47:ILE:HA	2:A:99:MET:SD	2.59	0.43
4:S:25:DG:H2"	4:S:26:DT:C6	2.53	0.43
3:R:6112:ALA:CB	3:R:6115:VAL:HG22	2.49	0.43
3:P:7052:VAL:CG2	3:P:7053:ALA:N	2.81	0.43
3:Q:5118:ILE:HG22	3:Q:5169:LEU:HD13	2.01	0.43
1:E:59:VAL:O	1:E:63:LEU:HG	2.19	0.43
1:C:81:ILE:HD11	1:C:120:HIS:HB2	2.01	0.43
3:F:7124:GLN:OE1	3:F:7128:ARG:NH2	2.52	0.43
6:L:700:08T:H6	6:L:700:08T:N3	2.32	0.43
2:A:22:TRP:HA	2:A:25:VAL:HB	2.00	0.43
3:R:6027:GLN:HG2	3:R:6047:VAL:CA	2.41	0.43
3:G:5149:ILE:CG2	3:G:5150:ASN:N	2.81	0.43
3:P:7148:VAL:CG1	3:P:7168:THR:HG23	2.45	0.43
1:O:165:LYS:HG3	1:O:201:PHE:CE2	2.54	0.43
1:C:238:VAL:O	1:C:242:LEU:HD13	2.19	0.43
3:R:6060:PHE:HD2	3:R:6092:TRP:CG	2.37	0.43
3:R:6092:TRP:CG	3:R:6093:PRO:HD2	2.53	0.43
1:D:257:TYR:CD1	1:D:264:PHE:CD1	3.07	0.43
1:O:74:VAL:HG12	1:O:75:ASN:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:254:ALA:N	1:M:255:PRO:HD2	2.34	0.43
1:C:83:PHE:O	1:C:87:PRO:HD2	2.19	0.43
3:Q:5071:ALA:HB1	3:Q:5084:ALA:O	2.19	0.43
1:L:289:GLY:CA	2:K:85:ILE:CG2	2.97	0.43
2:K:62:LYS:HE3	2:K:91:ASP:OD1	2.18	0.43
1:N:38:SER:C	1:N:40:GLY:N	2.72	0.43
1:B:269:ALA:HA	1:B:284:MET:HE1	2.01	0.43
3:P:7076:SER:HB2	3:P:7082:LYS:HB2	2.01	0.43
2:K:19:SER:O	2:K:20:LYS:HB2	2.19	0.43
3:G:5198:LEU:HD12	3:G:5198:LEU:O	2.19	0.43
3:H:6050:PHE:HD1	3:H:6050:PHE:N	2.16	0.43
1:E:94:ALA:O	1:E:102:LYS:HE3	2.19	0.43
3:Q:5002:LYS:HE2	3:Q:5070:ASP:O	2.19	0.43
3:Q:5109:PHE:HA	3:Q:5110:PRO:HD2	1.78	0.43
1:O:254:ALA:N	1:O:255:PRO:HD2	2.33	0.43
3:F:7106:PRO:O	3:F:7107:ILE:C	2.57	0.43
1:L:48:HIS:NE2	1:L:141:ILE:HD11	2.29	0.42
3:Q:5157:ASP:OD1	3:Q:5161:THR:N	2.48	0.42
3:H:6092:TRP:CG	3:H:6093:PRO:HD2	2.54	0.42
3:P:7061:LEU:HA	3:P:7064:LEU:HD12	2.01	0.42
1:B:165:LYS:HB2	1:B:165:LYS:HE3	1.83	0.42
2:K:105:GLY:O	2:K:106:LYS:HB2	2.19	0.42
1:L:204:PHE:O	1:L:207:THR:HG22	2.19	0.42
1:L:165:LYS:HE3	1:L:165:LYS:HB2	1.84	0.42
1:L:88:LEU:HA	1:L:88:LEU:HD12	1.74	0.42
1:O:307:TYR:CD2	2:K:80:TYR:CE1	3.07	0.42
1:M:49:SER:N	1:M:56:LYS:HD3	2.34	0.42
3:Q:5038:THR:HG22	3:Q:5218:VAL:HG12	2.01	0.42
3:P:7031:THR:OG1	3:P:7032:ARG:N	2.52	0.42
1:C:49:SER:HB3	1:C:56:LYS:CE	2.48	0.42
1:B:276:VAL:HG23	1:B:318:TRP:HE3	1.83	0.42
1:E:12:GLU:O	8:E:700:ADP:O3'	2.32	0.42
3:R:6063:ILE:HG22	3:R:6063:ILE:O	2.20	0.42
3:F:7182:ILE:HD13	3:F:7218:VAL:CG2	2.49	0.42
1:B:185:ILE:HD13	1:B:215:SER:CB	2.49	0.42
2:K:105:GLY:O	2:K:106:LYS:HE2	2.18	0.42
2:K:39:GLU:OE2	2:K:58:LYS:HE2	2.18	0.42
3:Q:5024:LYS:HG2	3:Q:5051:ASP:CG	2.40	0.42
1:N:148:LEU:HD23	1:N:148:LEU:HA	1.77	0.42
1:C:76:GLY:N	1:C:107:ASP:O	2.50	0.42
1:D:303:LEU:HD22	1:E:265:VAL:HG11	1.97	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:246:ASP:OD1	1:N:246:ASP:N	2.49	0.42
1:D:256:LYS:CE	1:E:159:GLN:HE22	2.30	0.42
1:L:292:ASN:HD21	2:K:88:GLY:CA	2.30	0.42
1:O:247:VAL:HG21	2:K:73:PRO:HG3	2.01	0.42
1:E:183:GLU:HB3	1:E:185:ILE:HG13	2.00	0.42
3:F:7050:PHE:HE2	3:F:7074:SER:HA	1.84	0.42
1:C:247:VAL:O	1:C:248:LYS:C	2.56	0.42
1:L:94:ALA:HA	3:P:7095:ALA:HA	2.01	0.42
2:K:164:ASP:O	2:K:167:LEU:HB2	2.19	0.42
1:O:199:LYS:HB3	1:O:200:ASN:OD1	2.19	0.42
3:R:6003:LEU:CD2	3:R:6007:THR:HG21	2.43	0.42
3:P:7080:ASN:HA	3:P:7094:ALA:HB2	2.01	0.42
1:D:32:THR:O	1:D:36:ILE:HG13	2.19	0.42
1:N:291:ASN:ND2	1:N:304:HIS:CE1	2.88	0.42
2:A:117:ASP:OD2	2:A:119:THR:HB	2.19	0.42
1:E:312:LEU:HA	1:E:312:LEU:HD23	1.90	0.42
1:N:297:ILE:HG22	1:O:295:HIS:O	2.19	0.42
1:B:289:GLY:C	2:A:85:ILE:HG23	2.40	0.42
3:G:5135:ILE:HA	3:G:5152:PHE:O	2.19	0.42
3:G:5135:ILE:O	3:G:5184:MSE:HG3	2.20	0.42
1:M:141:ILE:C	1:M:143:GLY:N	2.73	0.42
2:A:28:ALA:O	2:A:31:SER:HB3	2.19	0.42
3:H:6107:ILE:HA	3:H:6108:PRO:HD3	1.75	0.42
1:D:94:ALA:O	1:D:102:LYS:HE3	2.19	0.42
1:E:199:LYS:HB3	1:E:200:ASN:OD1	2.19	0.42
1:O:24:ILE:O	8:O:700:ADP:N6	2.52	0.42
3:R:6053:ALA:HB3	3:R:6095:ALA:O	2.20	0.42
2:A:151:LEU:N	2:A:152:PRO:CD	2.83	0.42
3:G:5011:LEU:HB2	3:G:5061:LEU:HD11	2.01	0.42
1:D:250:LEU:HA	1:D:250:LEU:HD23	1.81	0.42
1:D:189:ASP:OD2	1:D:191:LYS:HE2	2.20	0.42
3:Q:5040:ALA:HB2	3:Q:5216:TYR:HD1	1.81	0.42
3:R:6017:ILE:HG12	3:R:6188:LYS:HD3	2.01	0.42
1:D:17:PRO:HB3	1:D:22:GLU:HB3	2.00	0.42
3:G:5025:SER:HA	3:G:5048:ILE:O	2.18	0.42
1:M:55:GLY:O	1:M:59:VAL:HG23	2.20	0.42
3:Q:5125:GLN:O	3:Q:5125:GLN:HG2	2.19	0.42
2:K:136:ASN:N	2:K:136:ASN:OD1	2.51	0.42
3:Q:5076:SER:HB3	3:Q:5078:ASP:HB3	2.01	0.42
1:D:251:ARG:CG	1:D:251:ARG:NH1	2.81	0.42
1:D:251:ARG:HH21	1:E:270:GLU:HA	1.78	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:102:VAL:O	2:A:102:VAL:HG22	2.20	0.42
1:B:120:HIS:ND1	2:A:29:ALA:HB2	2.34	0.42
3:P:7165:TYR:CG	3:P:7166:SER:N	2.87	0.42
3:Q:5011:LEU:HB2	3:Q:5061:LEU:HD21	2.01	0.42
3:F:7153:ASN:O	3:F:7157:ASP:HB2	2.20	0.42
3:G:5034:VAL:HG23	3:G:5101:VAL:CG2	2.48	0.42
1:M:15:TYR:O	1:M:17:PRO:HD3	2.19	0.42
3:G:5066:LEU:HD12	3:H:6129:VAL:CG2	2.50	0.42
3:P:7143:LYS:HE3	3:P:7143:LYS:HB2	1.71	0.42
2:K:89:LEU:O	2:K:90:SER:C	2.58	0.42
1:M:53:GLY:HA2	6:M:700:08T:O3A	2.20	0.42
1:N:250:LEU:HD23	1:N:250:LEU:HA	1.82	0.42
1:O:81:ILE:HG23	1:O:82:ASP:N	2.34	0.42
1:C:16:ARG:NH2	6:C:700:08T:H2	2.35	0.42
3:G:5189:MSE:CB	3:G:5216:TYR:CD2	2.95	0.42
1:M:318:TRP:O	1:M:319:LYS:HG2	2.19	0.42
2:A:145:LEU:HB3	2:A:151:LEU:HB3	2.00	0.42
3:R:6115:VAL:CG1	3:R:6195:LYS:HE2	2.49	0.42
3:R:6067:VAL:HG13	3:R:6085:ASP:OD2	2.19	0.42
1:D:238:VAL:O	1:D:242:LEU:HD13	2.20	0.42
3:Q:5200:ALA:CB	3:Q:5226:HIS:NE2	2.82	0.42
3:F:7152:PHE:CB	3:F:7160:LEU:HD22	2.49	0.42
5:J:12:DG:H2"	5:J:13:DA:O5'	2.18	0.42
5:T:15:DT:N3	5:T:16:DA:C5	2.88	0.42
1:C:254:ALA:N	1:C:255:PRO:HD2	2.34	0.42
1:M:176:LEU:HD22	1:M:211:LEU:HD22	2.00	0.42
1:B:97:PHE:N	1:B:97:PHE:CD1	2.87	0.42
1:D:298:ALA:HA	1:E:292:ASN:O	2.20	0.42
1:D:111:ARG:NH2	4:I:15:DT:OP1	2.32	0.42
3:H:6090:ILE:HG23	3:F:7133:LEU:HD11	2.02	0.42
3:P:7046:ASP:N	3:P:7046:ASP:OD1	2.50	0.42
2:K:109:GLY:CA	4:S:8:DT:O4'	2.59	0.42
2:K:61:SER:O	2:K:65:VAL:HG23	2.18	0.42
2:A:125:LYS:HB3	2:A:166:PHE:CZ	2.55	0.42
1:D:213:SER:HB3	1:E:153:ARG:NE	2.35	0.42
3:Q:5116:THR:HB	3:Q:5147:ILE:CD1	2.49	0.42
1:E:141:ILE:HG22	1:E:149:GLN:NE2	2.34	0.42
1:D:67:VAL:CG1	1:D:67:VAL:O	2.66	0.42
1:O:59:VAL:O	1:O:59:VAL:HG12	2.20	0.42
1:E:102:LYS:O	1:E:132:CYS:HA	2.20	0.42
1:N:185:ILE:HD13	1:N:215:SER:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:7050:PHE:CZ	3:F:7074:SER:C	2.93	0.42
3:Q:5160:LEU:HD23	3:Q:5160:LEU:N	2.33	0.42
4:I:28:DT:H6	4:I:28:DT:OP2	2.01	0.42
2:A:40:PHE:CE2	2:A:64:MET:HG3	2.54	0.42
1:L:140:ASN:OD1	1:L:142:ASP:HB2	2.20	0.42
1:O:167:GLU:O	1:O:171:GLN:HG3	2.20	0.42
1:O:110:ASP:N	1:O:110:ASP:OD1	2.43	0.42
1:M:151:ARG:HH11	1:M:151:ARG:HG3	1.84	0.42
1:M:283:ARG:HD2	1:M:283:ARG:HA	1.94	0.42
2:K:167:LEU:HD13	2:K:180:LEU:HG	2.02	0.42
1:C:303:LEU:CD2	1:D:265:VAL:HG11	2.49	0.42
1:C:72:MET:HE3	1:C:72:MET:HB2	1.91	0.42
3:R:6001:MSE:HG3	3:R:6001:MSE:O	2.19	0.42
3:R:6179:ASN:HB3	3:R:6225:THR:CG2	2.44	0.42
5:T:6:DC:H2"	5:T:7:DA:O5'	2.19	0.42
1:M:3:THR:N	1:M:22:GLU:OE2	2.45	0.42
1:M:3:THR:HG21	1:M:18:SER:HB2	2.02	0.42
3:R:6190:GLN:HA	3:R:6191:PRO:HD3	1.88	0.42
2:A:63:PHE:CD1	2:A:63:PHE:C	2.93	0.42
3:R:6014:PHE:CE1	3:R:6040:ALA:HB1	2.55	0.42
3:G:5212:GLU:H	3:G:5212:GLU:HG2	1.63	0.42
1:L:156:THR:HG21	1:L:159:GLN:HE21	1.85	0.42
1:L:159:GLN:HA	1:L:160:PRO:HD2	1.94	0.42
1:D:141:ILE:C	1:D:143:GLY:N	2.73	0.41
1:N:48:HIS:HA	1:N:138:ALA:O	2.20	0.41
3:F:7024:LYS:HE3	3:F:7024:LYS:HB2	1.88	0.41
3:R:6200:ALA:HB3	3:R:6226:HIS:CD2	2.55	0.41
5:J:4:DG:H3'	5:J:4:DG:P	2.60	0.41
2:K:120:GLU:HG3	2:K:142:LYS:HZ1	1.84	0.41
2:K:152:PRO:CD	2:K:153:LEU:N	2.83	0.41
2:K:145:LEU:HD13	2:K:154:VAL:HG21	2.02	0.41
3:R:6138:ILE:CG2	3:R:6184:MSE:HE3	2.49	0.41
2:A:162:VAL:O	2:A:163:THR:C	2.57	0.41
2:K:40:PHE:CE2	2:K:64:MET:HG3	2.55	0.41
3:G:5011:LEU:HD21	3:G:5029:ILE:HD13	2.01	0.41
2:K:122:LEU:HD22	2:K:126:LEU:HD11	2.03	0.41
1:N:29:ASP:HA	1:N:32:THR:CG2	2.46	0.41
3:G:5016:THR:HB	3:G:5188:LYS:HD2	2.01	0.41
1:O:196:LEU:HA	1:O:196:LEU:HD23	1.75	0.41
1:B:120:HIS:ND1	2:A:29:ALA:CB	2.84	0.41
5:J:3:DA:C2'	5:J:4:DG:OP2	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:5076:SER:C	3:G:5078:ASP:N	2.71	0.41
1:E:81:ILE:HG23	1:E:82:ASP:N	2.34	0.41
1:O:56:LYS:HA	1:O:157:PHE:CE2	2.50	0.41
1:L:242:LEU:HD12	1:L:250:LEU:HD11	2.01	0.41
4:S:27:DC:C2'	4:S:28:DT:H71	2.49	0.41
2:A:136:ASN:OD1	2:A:136:ASN:N	2.50	0.41
3:R:6054:ILE:HG22	3:R:6056:ASP:O	2.20	0.41
3:F:7147:ILE:O	3:F:7169:LEU:HD12	2.20	0.41
1:E:124:PHE:O	1:E:127:ALA:N	2.53	0.41
1:N:201:PHE:HB3	1:N:202:PRO:HD3	2.03	0.41
3:F:7116:THR:HG22	3:F:7196:LEU:HD23	2.02	0.41
1:B:176:LEU:HA	1:B:176:LEU:HD23	1.78	0.41
1:B:204:PHE:O	1:B:207:THR:HG22	2.20	0.41
3:P:7011:LEU:HD11	3:P:7029:ILE:HD13	2.02	0.41
1:L:81:ILE:HD13	1:L:116:GLU:HG3	2.01	0.41
3:R:6002:LYS:HE2	3:R:6072:GLU:OE1	2.19	0.41
2:A:126:LEU:HG	2:A:166:PHE:CZ	2.55	0.41
1:B:100:ARG:O	1:B:101:GLN:C	2.58	0.41
1:N:230:ASN:O	1:N:232:ARG:N	2.53	0.41
1:C:307:TYR:CE1	1:D:286:GLU:HA	2.56	0.41
3:Q:5138:ILE:HA	3:Q:5150:ASN:O	2.20	0.41
1:M:201:PHE:O	1:M:203:ASP:N	2.53	0.41
2:A:19:SER:O	2:A:20:LYS:HB2	2.20	0.41
1:O:96:SER:HB3	1:O:102:LYS:HE2	2.03	0.41
1:D:200:ASN:HD21	1:D:210:GLU:HG3	1.85	0.41
3:G:5183:ASN:HB2	3:G:5221:GLU:CD	2.40	0.41
1:O:257:TYR:CD1	1:O:264:PHE:CD1	3.08	0.41
1:M:64:CYS:HB3	1:M:69:ALA:HB3	2.02	0.41
3:P:7109:PHE:HD2	3:P:7208:LYS:CD	2.22	0.41
3:F:7138:ILE:HG22	3:F:7151:GLY:HA2	2.02	0.41
3:P:7162:ARG:CG	3:P:7162:ARG:NH1	2.81	0.41
1:O:201:PHE:HB3	1:O:202:PRO:HD3	2.02	0.41
1:D:213:SER:HB3	1:E:153:ARG:NH1	2.36	0.41
1:N:224:ILE:O	1:N:228:VAL:HG23	2.20	0.41
3:Q:5221:GLU:O	3:Q:5222:ALA:C	2.59	0.41
1:L:67:VAL:O	1:L:68:ASN:C	2.59	0.41
3:Q:5067:VAL:HG23	3:Q:5068:ASN:N	2.35	0.41
1:B:74:VAL:HG21	1:B:83:PHE:HE2	1.86	0.41
3:F:7105:LYS:HA	3:F:7106:PRO:HD3	1.88	0.41
1:N:200:ASN:HD21	1:N:210:GLU:HG3	1.84	0.41
1:M:257:TYR:CD1	1:M:264:PHE:CD1	3.09	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:158:GLY:O	1:B:160:PRO:HD3	2.20	0.41
1:O:251:ARG:NE	2:K:71:GLN:CD	2.57	0.41
1:O:219:VAL:HG12	1:O:220:LEU:N	2.35	0.41
3:G:5149:ILE:HG13	3:G:5169:LEU:HD11	2.03	0.41
3:G:5063:ILE:O	3:G:5063:ILE:CG2	2.69	0.41
1:D:25:LEU:CD2	1:D:157:PHE:HE2	2.31	0.41
1:L:310:ILE:CD1	1:M:285:TYR:HD2	2.32	0.41
1:N:214:TYR:O	1:N:224:ILE:HD13	2.20	0.41
1:B:62:ALA:O	1:B:63:LEU:C	2.56	0.41
1:L:96:SER:O	1:L:96:SER:OG	2.37	0.41
1:N:176:LEU:HD22	1:N:211:LEU:HD22	2.01	0.41
3:P:7063:ILE:HG13	3:P:7092:TRP:HZ3	1.85	0.41
1:E:64:CYS:SG	1:E:103:VAL:HG11	2.60	0.41
2:K:75:CYS:O	2:K:79:VAL:HG23	2.20	0.41
3:G:5210:GLU:HG3	3:G:5215:ASN:HD21	1.85	0.41
3:P:7030:MSE:HE1	3:P:7106:PRO:CA	2.51	0.41
3:P:7030:MSE:SE	3:P:7103:PRO:HB2	2.70	0.41
1:D:97:PHE:CE2	3:G:5078:ASP:O	2.73	0.41
2:K:114:LEU:HA	2:K:114:LEU:HD23	1.71	0.41
3:G:5128:ARG:HB3	3:F:7066:LEU:CD1	2.49	0.41
1:B:307:TYR:CE2	1:C:293:GLN:OE1	2.74	0.41
1:L:30:LYS:O	1:L:34:LYS:HG2	2.19	0.41
1:N:64:CYS:HB3	1:N:69:ALA:HB3	2.03	0.41
3:R:6143:LYS:HB3	3:R:6148:VAL:HG11	2.03	0.41
1:D:44:HIS:CE1	1:D:133:SER:HA	2.55	0.41
1:L:231:ASP:OD1	1:L:231:ASP:O	2.38	0.41
2:K:72:PHE:N	2:K:72:PHE:CD1	2.89	0.41
1:C:139:ASN:HD22	1:D:122:ARG:HE	1.67	0.41
3:R:6178:PHE:HB3	3:R:6226:HIS:HB2	2.03	0.41
1:L:81:ILE:CG2	1:L:82:ASP:N	2.83	0.41
3:F:7004:SER:O	3:F:7005:LYS:C	2.58	0.41
6:B:700:08T:H6	6:B:700:08T:N3	2.28	0.41
1:B:179:ILE:HG21	1:B:179:ILE:HD13	1.77	0.41
2:K:162:VAL:O	2:K:163:THR:C	2.58	0.41
3:G:5092:TRP:CD1	3:G:5093:PRO:N	2.87	0.41
3:G:5128:ARG:HD3	3:F:7066:LEU:HD21	2.03	0.41
3:H:6088:SER:HB2	3:F:7166:SER:O	2.21	0.41
1:D:154:VAL:HG12	1:D:154:VAL:O	2.19	0.41
1:L:23:CYS:O	1:L:30:LYS:HE2	2.21	0.41
3:F:7117:GLU:HG2	3:F:7118:ILE:N	2.35	0.41
3:F:7096:ASP:OD2	3:F:7098:SER:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:141:ILE:HD13	1:D:141:ILE:HG21	1.72	0.41
3:Q:5210:GLU:CG	3:Q:5215:ASN:HD21	2.33	0.41
3:H:6139:ALA:HA	3:H:6180:PHE:O	2.20	0.41
3:H:6161:THR:OG1	3:H:6162:ARG:N	2.54	0.41
3:Q:5133:LEU:HD22	3:Q:5164:LYS:HD3	2.03	0.41
2:K:20:LYS:HE3	3:P:7055:TYR:CZ	2.55	0.41
1:L:63:LEU:HD23	1:L:63:LEU:HA	1.76	0.41
3:P:7150:ASN:HB3	3:P:7163:VAL:HG23	2.03	0.41
1:C:255:PRO:HA	1:C:302:GLU:HG3	2.03	0.41
1:E:297:ILE:HD13	1:E:297:ILE:HG21	1.86	0.41
2:K:4:PHE:HZ	3:P:7039:TYR:HD2	1.69	0.41
2:A:102:VAL:HG21	2:A:104:ARG:HH21	1.86	0.41
1:D:295:HIS:ND1	1:D:296:GLY:N	2.69	0.41
1:D:119:ARG:CB	1:D:122:ARG:NH1	2.84	0.41
4:I:8:DT:H2"	4:I:9:DT:H5'	2.03	0.41
3:R:6150:ASN:CB	3:R:6152:PHE:CE1	3.04	0.41
1:C:97:PHE:HD2	3:G:5199:TRP:HZ3	1.69	0.41
3:R:6085:ASP:HB3	3:R:6088:SER:O	2.20	0.41
3:F:7018:ASN:C	3:F:7020:GLY:H	2.23	0.41
3:Q:5223:ASP:O	3:Q:5224:SER:C	2.59	0.41
1:C:47:LEU:HD22	1:C:157:PHE:CE1	2.51	0.41
1:C:33:PHE:CZ	1:C:155:ILE:HD13	2.56	0.41
4:S:23:DG:C2	4:S:24:DT:C2	3.09	0.41
1:M:242:LEU:CD1	1:M:250:LEU:HD21	2.49	0.41
3:R:6050:PHE:CE2	3:R:6075:GLN:HB3	2.55	0.41
1:M:67:VAL:CG1	1:M:67:VAL:O	2.67	0.41
3:R:6107:ILE:HG23	3:R:6108:PRO:HD2	2.02	0.41
1:B:93:SER:HA	3:F:7099:THR:HG21	2.02	0.41
1:E:196:LEU:HA	1:E:196:LEU:HD23	1.75	0.41
2:K:85:ILE:O	2:K:85:ILE:CG2	2.69	0.41
1:L:293:GLN:NE2	2:K:84:LEU:C	2.65	0.41
3:Q:5128:ARG:HH22	4:S:29:DG:H5"	1.84	0.41
1:N:275:ARG:O	1:N:318:TRP:HB2	2.21	0.41
1:N:285:TYR:HD1	1:N:285:TYR:HA	1.68	0.41
1:D:94:ALA:HA	3:G:5095:ALA:HA	2.03	0.41
1:D:285:TYR:HA	1:D:285:TYR:HD1	1.69	0.41
2:K:159:LYS:HG3	2:K:160:GLY:N	2.35	0.41
3:P:7023:LEU:HD11	3:P:7052:VAL:HG13	2.03	0.41
3:R:6066:LEU:HD12	3:R:6067:VAL:H	1.85	0.41
1:M:238:VAL:O	1:M:242:LEU:HD13	2.21	0.41
3:G:5092:TRP:HA	3:G:5093:PRO:HD3	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:5048:ILE:N	3:Q:5048:ILE:HD12	2.36	0.41
1:E:111:ARG:CG	1:E:112:SER:N	2.45	0.40
1:D:48:HIS:HA	1:D:138:ALA:O	2.21	0.40
3:F:7133:LEU:HB3	3:F:7164:LYS:HZ3	1.85	0.40
3:F:7022:MSE:HB2	3:F:7102:ALA:CB	2.50	0.40
3:R:6146:LYS:CA	3:R:6171:ASP:HA	2.37	0.40
1:M:239:LEU:O	1:M:243:LYS:HG3	2.21	0.40
3:H:6021:ILE:HG13	3:H:6031:THR:OG1	2.21	0.40
3:P:7041:GLU:O	3:P:7042:ALA:HB2	2.21	0.40
1:O:243:LYS:HE2	1:O:318:TRP:HE1	1.87	0.40
2:K:139:ILE:O	2:K:140:ASN:C	2.60	0.40
1:O:238:VAL:O	1:O:242:LEU:HD13	2.21	0.40
1:O:124:PHE:O	1:O:127:ALA:N	2.52	0.40
1:B:307:TYR:HE2	1:C:293:GLN:OE1	2.04	0.40
1:E:257:TYR:CD1	1:E:264:PHE:CD1	3.09	0.40
1:O:46:ILE:HG13	1:O:152:CYS:HB3	2.04	0.40
1:C:48:HIS:ND1	1:C:141:ILE:CG1	2.84	0.40
4:I:17:DC:N4	5:J:14:DG:H1	2.12	0.40
3:P:7010:LEU:HD12	3:P:7044:ILE:HD13	2.03	0.40
2:A:4:PHE:CD2	3:F:7032:ARG:NH1	2.90	0.40
1:N:49:SER:HB3	1:N:56:LYS:CE	2.49	0.40
1:O:12:GLU:HG3	1:O:13:GLN:N	2.36	0.40
1:L:120:HIS:ND1	2:K:29:ALA:HB2	2.36	0.40
1:B:121:LEU:O	1:B:124:PHE:N	2.54	0.40
1:D:165:LYS:HG2	1:D:169:MET:HE3	2.02	0.40
3:Q:5118:ILE:CG1	3:Q:5118:ILE:O	2.64	0.40
1:N:32:THR:O	1:N:36:ILE:HG13	2.22	0.40
1:N:47:LEU:HD22	1:N:157:PHE:CE1	2.52	0.40
1:O:87:PRO:O	1:O:90:ASN:N	2.54	0.40
1:B:186:ALA:HB3	1:B:219:VAL:HG23	2.03	0.40
1:D:38:SER:O	1:D:39:LYS:C	2.60	0.40
1:B:307:TYR:CG	1:C:289:GLY:HA3	2.56	0.40
1:B:304:HIS:CE1	1:C:293:GLN:HG2	2.57	0.40
3:Q:5024:LYS:HG2	3:Q:5051:ASP:CB	2.51	0.40
3:P:7063:ILE:HA	3:P:7063:ILE:HD13	1.92	0.40
1:B:147:PRO:HG2	2:A:32:PHE:HB3	2.03	0.40
3:P:7047:VAL:O	3:P:7047:VAL:HG23	2.22	0.40
1:C:2:ILE:CG2	1:C:3:THR:N	2.83	0.40
2:K:4:PHE:O	2:K:6:ASP:N	2.54	0.40
2:A:29:ALA:C	2:A:31:SER:N	2.75	0.40
3:P:7105:LYS:HZ3	3:P:7107:ILE:CD1	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:6080:ASN:HA	3:H:6094:ALA:HB3	2.02	0.40
3:R:6011:LEU:C	3:R:6061:LEU:HD11	2.42	0.40
3:Q:5118:ILE:HD11	3:Q:5123:LEU:HB2	2.02	0.40
3:R:6120:ALA:CB	3:R:6192:GLY:HA2	2.51	0.40
1:B:285:TYR:HD1	1:B:285:TYR:HA	1.72	0.40
1:M:9:HIS:CD2	1:N:41:LYS:CB	3.04	0.40
3:R:6157:ASP:OD2	3:R:6161:THR:N	2.54	0.40
3:Q:5135:ILE:HA	3:Q:5152:PHE:O	2.21	0.40
2:K:23:THR:HA	2:K:26:GLN:HB2	2.03	0.40
3:Q:5102:ALA:HA	3:Q:5103:PRO:HD3	1.74	0.40
3:Q:5141:THR:OG1	3:Q:5142:VAL:N	2.54	0.40
1:M:49:SER:OG	1:M:50:PRO:HA	2.21	0.40
1:O:251:ARG:HH12	2:K:70:SER:HG	1.55	0.40
1:E:145:ILE:H	1:E:145:ILE:HG23	1.56	0.40
1:D:95:ALA:CA	3:G:5096:ASP:HB3	2.50	0.40
1:E:200:ASN:HD22	1:E:206:LYS:CG	2.23	0.40
3:R:6081:ILE:O	3:R:6091:PHE:HA	2.21	0.40
3:R:6011:LEU:HA	3:R:6011:LEU:HD23	1.99	0.40
3:P:7153:ASN:O	3:P:7157:ASP:CB	2.64	0.40
2:A:64:MET:SD	4:I:10:DT:C2	3.14	0.40
1:L:190:MET:C	1:L:192:VAL:N	2.75	0.40
1:B:192:VAL:HG12	1:B:193:VAL:N	2.36	0.40
5:T:7:DA:H2"	5:T:8:DC:H6	1.86	0.40
1:B:80:LYS:C	1:B:117:SER:OG	2.60	0.40
3:R:6147:ILE:O	3:R:6147:ILE:HG13	2.20	0.40
4:S:16:DA:C2	4:S:17:DC:C2	3.10	0.40
1:D:64:CYS:HB3	1:D:69:ALA:HB3	2.02	0.40
2:K:82:MET:HB3	2:K:94:HIS:HE2	1.86	0.40
1:O:20:ILE:CG2	1:O:34:LYS:NZ	2.85	0.40
1:O:51:SER:O	1:O:54:THR:HG23	2.22	0.40
3:P:7117:GLU:O	3:P:7169:LEU:HD22	2.22	0.40
1:C:141:ILE:O	1:C:143:GLY:N	2.55	0.40
2:K:102:VAL:HG21	2:K:104:ARG:HH21	1.86	0.40
1:B:116:GLU:O	1:B:120:HIS:HB2	2.22	0.40
1:L:316:MET:CB	1:L:318:TRP:CZ3	3.04	0.40
2:K:146:THR:HG22	2:K:151:LEU:HD23	2.03	0.40
3:P:7023:LEU:HB2	3:P:7048:ILE:HD13	2.03	0.40
2:A:38:ASN:HB3	4:I:9:DT:C7	2.51	0.40
1:C:272:ILE:O	1:C:276:VAL:HG12	2.21	0.40
3:R:6067:VAL:CG2	3:R:6090:ILE:HD12	2.52	0.40
3:G:5011:LEU:HB3	3:G:5061:LEU:HD11	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:90:ASN:HA	3:F:7055:TYR:CE2	2.56	0.40
3:H:6136:ASP:O	3:H:6184:MSE:HB2	2.22	0.40
3:P:7003:LEU:HA	3:P:7003:LEU:HD23	1.82	0.40
1:L:282:ILE:O	1:L:286:GLU:HG3	2.22	0.40
1:M:251:ARG:HH21	1:N:270:GLU:HG3	1.86	0.40
1:B:71:MET:HE2	1:B:105:VAL:HG21	2.03	0.40
1:D:8:GLU:OE2	1:D:13:GLN:HG2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	318/324 (98%)	303 (95%)	15 (5%)	0	100	100
1	C	318/324 (98%)	296 (93%)	22 (7%)	0	100	100
1	D	318/324 (98%)	295 (93%)	23 (7%)	0	100	100
1	E	301/324 (93%)	277 (92%)	23 (8%)	1 (0%)	46	84
1	L	318/324 (98%)	301 (95%)	17 (5%)	0	100	100
1	M	318/324 (98%)	297 (93%)	21 (7%)	0	100	100
1	N	318/324 (98%)	294 (92%)	24 (8%)	0	100	100
1	O	301/324 (93%)	276 (92%)	25 (8%)	0	100	100
2	A	184/199 (92%)	155 (84%)	26 (14%)	3 (2%)	12	55
2	K	184/199 (92%)	153 (83%)	28 (15%)	3 (2%)	12	55
3	F	226/228 (99%)	211 (93%)	14 (6%)	1 (0%)	39	81
3	G	226/228 (99%)	209 (92%)	16 (7%)	1 (0%)	39	81
3	H	226/228 (99%)	211 (93%)	13 (6%)	2 (1%)	21	68
3	P	226/228 (99%)	203 (90%)	23 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	Q	226/228 (99%)	211 (93%)	15 (7%)	0	100 100
3	R	226/228 (99%)	206 (91%)	18 (8%)	2 (1%)	21 68
All	All	4234/4358 (97%)	3898 (92%)	323 (8%)	13 (0%)	46 84

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	8	ILE
3	H	6079	GLY
3	R	6111	VAL
2	A	151	LEU
3	G	5057	LEU
3	F	7086	ALA
2	K	151	LEU
3	R	6191	PRO
1	E	199	LYS
2	A	103	PRO
3	H	6110	PRO
2	K	8	ILE
2	K	103	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	278/279 (100%)	258 (93%)	20 (7%)	18 57
1	C	278/279 (100%)	263 (95%)	15 (5%)	27 67
1	D	278/279 (100%)	267 (96%)	11 (4%)	38 75
1	E	266/279 (95%)	245 (92%)	21 (8%)	15 53
1	L	278/279 (100%)	258 (93%)	20 (7%)	18 57
1	M	278/279 (100%)	266 (96%)	12 (4%)	35 74
1	N	278/279 (100%)	265 (95%)	13 (5%)	32 72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	O	266/279 (95%)	246 (92%)	20 (8%)	17 55
2	A	161/174 (92%)	137 (85%)	24 (15%)	4 22
2	K	161/174 (92%)	138 (86%)	23 (14%)	4 24
3	F	189/183 (103%)	169 (89%)	20 (11%)	8 38
3	G	189/183 (103%)	169 (89%)	20 (11%)	8 38
3	H	189/183 (103%)	169 (89%)	20 (11%)	8 38
3	P	189/183 (103%)	171 (90%)	18 (10%)	11 43
3	Q	189/183 (103%)	173 (92%)	16 (8%)	13 49
3	R	189/183 (103%)	175 (93%)	14 (7%)	17 56
All	All	3656/3678 (99%)	3369 (92%)	287 (8%)	15 53

All (287) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	0	SER
1	B	2	ILE
1	B	16	ARG
1	B	32	THR
1	B	81	ILE
1	B	89	THR
1	B	98	ASP
1	B	114	LEU
1	B	120	HIS
1	B	129	SER
1	B	146	LYS
1	B	148	LEU
1	B	150	SER
1	B	156	THR
1	B	162	ASP
1	B	173	ILE
1	B	200	ASN
1	B	207	THR
1	B	251	ARG
1	B	277	THR
1	C	0	SER
1	C	9	HIS
1	C	16	ARG
1	C	77	SER
1	C	81	ILE

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Mol	Chain	Res	Type
1	C	109	PHE
1	C	140	ASN
1	C	200	ASN
1	C	207	THR
1	C	216	SER
1	C	232	ARG
1	C	251	ARG
1	C	277	THR
1	C	317	GLN
1	C	318	TRP
1	D	0	SER
1	D	9	HIS
1	D	16	ARG
1	D	77	SER
1	D	78	ASP
1	D	81	ILE
1	D	109	PHE
1	D	200	ASN
1	D	207	THR
1	D	216	SER
1	D	277	THR
1	E	3	THR
1	E	8	GLU
1	E	11	LEU
1	E	32	THR
1	E	77	SER
1	E	79	CYS
1	E	88	LEU
1	E	101	GLN
1	E	109	PHE
1	E	114	LEU
1	E	117	SER
1	E	122	ARG
1	E	123	SER
1	E	132	CYS
1	E	154	VAL
1	E	161	THR
1	E	199	LYS
1	E	200	ASN
1	E	207	THR
1	E	251	ARG
1	E	277	THR

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Mol	Chain	Res	Type
2	A	2	SER
2	A	3	LEU
2	A	23	THR
2	A	39	GLU
2	A	55	ILE
2	A	58	LYS
2	A	59	ASP
2	A	70	SER
2	A	74	GLU
2	A	89	LEU
2	A	91	ASP
2	A	102	VAL
2	A	104	ARG
2	A	108	TYR
2	A	122	LEU
2	A	135	THR
2	A	136	ASN
2	A	143	SER
2	A	151	LEU
2	A	156	LYS
2	A	161	LEU
2	A	176	GLU
2	A	180	LEU
2	A	183	LEU
3	G	5004	SER
3	G	5006	ASP
3	G	5023	LEU
3	G	5029	ILE
3	G	5034	VAL
3	G	5044	ILE
3	G	5045	SER
3	G	5054	ILE
3	G	5088	SER
3	G	5098	SER
3	G	5109	PHE
3	G	5111	VAL
3	G	5116	THR
3	G	5155	VAL
3	G	5158	SER
3	G	5161	THR
3	G	5163	VAL
3	G	5189	MSE

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Mol	Chain	Res	Type
3	G	5212	GLU
3	G	5221	GLU
3	H	6002	LYS
3	H	6007	THR
3	H	6010	LEU
3	H	6019	SER
3	H	6022	MSE
3	H	6023	LEU
3	H	6031	THR
3	H	6037	THR
3	H	6050	PHE
3	H	6063	ILE
3	H	6075	GLN
3	H	6078	ASP
3	H	6141	THR
3	H	6148	VAL
3	H	6152	PHE
3	H	6157	ASP
3	H	6158	SER
3	H	6166	SER
3	H	6171	ASP
3	H	6189	MSE
3	F	7029	ILE
3	F	7031	THR
3	F	7038	THR
3	F	7039	TYR
3	F	7043	ASN
3	F	7044	ILE
3	F	7089	THR
3	F	7109	PHE
3	F	7115	VAL
3	F	7117	GLU
3	F	7121	GLU
3	F	7137	THR
3	F	7143	LYS
3	F	7155	VAL
3	F	7175	GLU
3	F	7183	ASN
3	F	7189	MSE
3	F	7218	VAL
3	F	7220	LEU
3	F	7221	GLU

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Mol	Chain	Res	Type
1	L	2	ILE
1	L	9	HIS
1	L	16	ARG
1	L	32	THR
1	L	34	LYS
1	L	81	ILE
1	L	89	THR
1	L	98	ASP
1	L	114	LEU
1	L	120	HIS
1	L	129	SER
1	L	146	LYS
1	L	148	LEU
1	L	150	SER
1	L	156	THR
1	L	162	ASP
1	L	173	ILE
1	L	207	THR
1	L	251	ARG
1	L	277	THR
1	M	2	ILE
1	M	16	ARG
1	M	77	SER
1	M	81	ILE
1	M	109	PHE
1	M	140	ASN
1	M	200	ASN
1	M	207	THR
1	M	216	SER
1	M	231	ASP
1	M	251	ARG
1	M	277	THR
1	N	0	SER
1	N	9	HIS
1	N	16	ARG
1	N	77	SER
1	N	81	ILE
1	N	109	PHE
1	N	140	ASN
1	N	200	ASN
1	N	207	THR
1	N	216	SER

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Mol	Chain	Res	Type
1	N	251	ARG
1	N	277	THR
1	N	284	MET
1	O	3	THR
1	O	8	GLU
1	O	11	LEU
1	O	32	THR
1	O	77	SER
1	O	79	CYS
1	O	88	LEU
1	O	101	GLN
1	O	109	PHE
1	O	114	LEU
1	O	117	SER
1	O	132	CYS
1	O	145	ILE
1	O	154	VAL
1	O	161	THR
1	O	199	LYS
1	O	200	ASN
1	O	207	THR
1	O	251	ARG
1	O	277	THR
2	K	2	SER
2	K	3	LEU
2	K	23	THR
2	K	39	GLU
2	K	55	ILE
2	K	58	LYS
2	K	59	ASP
2	K	70	SER
2	K	74	GLU
2	K	89	LEU
2	K	91	ASP
2	K	102	VAL
2	K	104	ARG
2	K	108	TYR
2	K	122	LEU
2	K	135	THR
2	K	136	ASN
2	K	143	SER
2	K	151	LEU

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Mol	Chain	Res	Type
2	K	156	LYS
2	K	161	LEU
2	K	180	LEU
2	K	183	LEU
3	Q	5023	LEU
3	Q	5025	SER
3	Q	5037	THR
3	Q	5052	VAL
3	Q	5054	ILE
3	Q	5067	VAL
3	Q	5104	ASN
3	Q	5118	ILE
3	Q	5123	LEU
3	Q	5157	ASP
3	Q	5161	THR
3	Q	5166	SER
3	Q	5187	MSE
3	Q	5189	MSE
3	Q	5217	VAL
3	Q	5223	ASP
3	R	6013	ASN
3	R	6025	SER
3	R	6030	MSE
3	R	6111	VAL
3	R	6116	THR
3	R	6137	THR
3	R	6147	ILE
3	R	6168	THR
3	R	6189	MSE
3	R	6197	LEU
3	R	6199	TRP
3	R	6201	LYS
3	R	6218	VAL
3	R	6225	THR
3	P	7019	SER
3	P	7023	LEU
3	P	7038	THR
3	P	7046	ASP
3	P	7052	VAL
3	P	7063	ILE
3	P	7069	ASP
3	P	7088	SER

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Mol	Chain	Res	Type
3	P	7104	ASN
3	P	7109	PHE
3	P	7118	ILE
3	P	7149	ILE
3	P	7156	GLU
3	P	7189	MSE
3	P	7204	GLN
3	P	7215	ASN
3	P	7225	THR
3	P	7227	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	159	GLN
1	B	292	ASN
1	B	304	HIS
1	C	9	HIS
1	C	101	GLN
1	C	120	HIS
1	C	139	ASN
1	C	295	HIS
1	C	304	HIS
1	C	317	GLN
1	D	101	GLN
1	D	295	HIS
1	E	120	HIS
1	E	159	GLN
1	E	293	GLN
1	E	295	HIS
2	A	57	GLN
3	G	5027	GLN
3	G	5124	GLN
3	G	5215	ASN
3	G	5226	HIS
3	H	6190	GLN
3	H	6215	ASN
3	F	7018	ASN
3	F	7134	GLN
3	F	7215	ASN
1	L	9	HIS
1	L	159	GLN

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Mol	Chain	Res	Type
1	L	292	ASN
1	M	101	GLN
1	M	120	HIS
1	M	139	ASN
1	N	101	GLN
1	N	293	GLN
1	N	295	HIS
1	N	317	GLN
1	O	120	HIS
1	O	159	GLN
1	O	295	HIS
2	K	57	GLN
3	Q	5215	ASN
3	R	6013	ASN
3	R	6027	GLN
3	R	6153	ASN
3	R	6176	ASN
3	R	6215	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 for Mogul analysis.

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	$\#\|Z\| > 2$
6	08T	B	700	7	26,33,33	2.91	13 (50%)	28,52,52	5.66	10 (35%)
6	08T	C	700	7	26,33,33	2.84	13 (50%)	28,52,52	4.84	11 (39%)
6	08T	D	700	-	26,33,33	2.76	13 (50%)	28,52,52	5.45	6 (21%)
8	ADP	E	700	7	22,29,29	1.01	1 (4%)	27,45,45	2.30	5 (18%)
6	08T	L	700	7	26,33,33	2.79	13 (50%)	28,52,52	5.64	10 (35%)
6	08T	M	700	-	26,33,33	2.90	12 (46%)	28,52,52	5.35	8 (28%)
6	08T	N	700	-	26,33,33	2.80	13 (50%)	28,52,52	5.64	4 (14%)
8	ADP	O	700	7	22,29,29	1.07	1 (4%)	27,45,45	2.08	6 (22%)

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
6	08T	B	700	7	-	0/12/38/38	0/3/3/3
6	08T	C	700	7	-	0/12/38/38	0/3/3/3
6	08T	D	700	-	-	0/12/38/38	0/3/3/3
8	ADP	E	700	7	-	0/12/32/32	0/3/3/3
6	08T	L	700	7	-	0/12/38/38	0/3/3/3
6	08T	M	700	-	-	0/12/38/38	0/3/3/3
6	08T	N	700	-	-	0/12/38/38	0/3/3/3
8	ADP	O	700	7	-	0/12/32/32	0/3/3/3

All (79) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	700	08T	F1-BE	-6.61	1.37	1.54
6	M	700	08T	F1-BE	-6.35	1.37	1.54
6	C	700	08T	F1-BE	-6.27	1.38	1.54
6	L	700	08T	F1-BE	-6.20	1.38	1.54
6	M	700	08T	F3-BE	-6.01	1.38	1.54
6	N	700	08T	F1-BE	-5.88	1.39	1.54
6	D	700	08T	F1-BE	-5.82	1.39	1.54
6	C	700	08T	F3-BE	-5.58	1.39	1.54
6	M	700	08T	F2-BE	-5.49	1.40	1.54
6	L	700	08T	F3-BE	-5.41	1.40	1.54
6	B	700	08T	F3-BE	-5.38	1.40	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	700	08T	F2-BE	-5.30	1.40	1.54
6	B	700	08T	F2-BE	-5.30	1.40	1.54
6	N	700	08T	F3-BE	-5.30	1.40	1.54
6	D	700	08T	F2-BE	-5.26	1.40	1.54
6	D	700	08T	F3-BE	-5.17	1.40	1.54
6	N	700	08T	C2'-C3'	-5.14	1.39	1.53
6	N	700	08T	F2-BE	-4.95	1.41	1.54
6	B	700	08T	C2'-C3'	-4.92	1.40	1.53
6	C	700	08T	C2'-C3'	-4.92	1.40	1.53
6	M	700	08T	C2'-C3'	-4.85	1.40	1.53
6	L	700	08T	F2-BE	-4.76	1.41	1.54
6	D	700	08T	C2'-C3'	-4.72	1.40	1.53
6	L	700	08T	C2'-C3'	-4.70	1.40	1.53
6	L	700	08T	PA-O5'	-3.55	1.48	1.60
6	B	700	08T	C3'-C4'	-3.55	1.43	1.53
6	B	700	08T	PA-O5'	-3.49	1.49	1.60
6	L	700	08T	C3'-C4'	-3.39	1.43	1.53
6	D	700	08T	C3'-C4'	-3.26	1.44	1.53
6	M	700	08T	C3'-C4'	-3.24	1.44	1.53
6	M	700	08T	PB-O3A	-3.22	1.53	1.60
6	N	700	08T	C3'-C4'	-3.18	1.44	1.53
6	C	700	08T	O4'-C4'	-3.17	1.37	1.45
6	L	700	08T	O4'-C4'	-3.15	1.37	1.45
6	C	700	08T	C3'-C4'	-3.13	1.44	1.53
6	B	700	08T	PB-O3A	-3.12	1.54	1.60
6	M	700	08T	PA-O5'	-2.94	1.50	1.60
6	M	700	08T	O4'-C4'	-2.93	1.38	1.45
6	B	700	08T	O4'-C4'	-2.93	1.38	1.45
6	C	700	08T	PA-O5'	-2.89	1.50	1.60
6	D	700	08T	PA-O5'	-2.84	1.51	1.60
6	D	700	08T	PB-O3A	-2.80	1.54	1.60
6	D	700	08T	O4'-C4'	-2.72	1.38	1.45
6	N	700	08T	PB-O3A	-2.35	1.55	1.60
6	N	700	08T	O4'-C4'	-2.34	1.39	1.45
6	L	700	08T	PB-O3A	-2.31	1.55	1.60
6	N	700	08T	PA-O5'	-2.21	1.53	1.60
6	C	700	08T	C5-N7	-2.20	1.31	1.39
6	L	700	08T	C5-N7	-2.20	1.32	1.39
6	B	700	08T	C5-N7	-2.12	1.32	1.39
6	C	700	08T	PB-O3A	-2.02	1.56	1.60
6	L	700	08T	C4-N3	2.04	1.38	1.35
6	D	700	08T	C2-N3	2.21	1.36	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	N	700	08T	C2-N3	2.32	1.36	1.32
6	N	700	08T	C4-N3	2.44	1.39	1.35
6	B	700	08T	PA-O1A	2.48	1.54	1.48
6	M	700	08T	PA-O1A	2.51	1.54	1.48
6	M	700	08T	C6-N6	2.52	1.42	1.34
6	B	700	08T	C6-N6	2.53	1.42	1.34
6	D	700	08T	PA-O1A	2.58	1.54	1.48
6	B	700	08T	C4-N3	2.65	1.39	1.35
6	C	700	08T	C6-N6	2.72	1.43	1.34
6	C	700	08T	PA-O1A	2.72	1.55	1.48
6	C	700	08T	C4-N3	2.77	1.39	1.35
6	D	700	08T	C4-N3	2.84	1.39	1.35
6	M	700	08T	C4-N3	2.88	1.39	1.35
6	L	700	08T	PA-O1A	2.88	1.55	1.48
6	N	700	08T	C6-N6	2.89	1.43	1.34
6	L	700	08T	C6-N6	2.91	1.43	1.34
8	E	700	ADP	C5-C4	3.06	1.47	1.40
6	D	700	08T	C6-N6	3.11	1.44	1.34
6	N	700	08T	PA-O1A	3.30	1.56	1.48
8	O	700	ADP	C5-C4	3.44	1.48	1.40
6	L	700	08T	PB-O2B	3.53	1.57	1.48
6	D	700	08T	PB-O2B	3.75	1.57	1.48
6	M	700	08T	PB-O2B	3.76	1.57	1.48
6	C	700	08T	PB-O2B	3.90	1.57	1.48
6	B	700	08T	PB-O2B	3.96	1.58	1.48
6	N	700	08T	PB-O2B	4.47	1.59	1.48

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	N	700	08T	C1'-N9-C4	-27.33	85.72	126.94
6	B	700	08T	C1'-N9-C4	-26.56	86.88	126.94
6	D	700	08T	C1'-N9-C4	-26.27	87.31	126.94
6	L	700	08T	C1'-N9-C4	-25.95	87.80	126.94
6	M	700	08T	C1'-N9-C4	-24.88	89.42	126.94
6	C	700	08T	C1'-N9-C4	-21.94	93.85	126.94
6	L	700	08T	N3-C2-N1	-10.76	120.66	128.89
6	B	700	08T	N3-C2-N1	-10.72	120.69	128.89
6	M	700	08T	N3-C2-N1	-10.29	121.01	128.89
6	N	700	08T	N3-C2-N1	-9.98	121.25	128.89
6	C	700	08T	N3-C2-N1	-9.35	121.74	128.89
6	D	700	08T	N3-C2-N1	-9.33	121.75	128.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	E	700	ADP	C2'-C1'-N9	-7.44	102.93	114.29
8	O	700	ADP	N3-C2-N1	-7.01	123.53	128.89
8	E	700	ADP	N3-C2-N1	-6.34	124.04	128.89
6	L	700	08T	O1A-PA-O2A	-4.20	106.20	118.70
8	O	700	ADP	C2'-C1'-N9	-4.02	108.15	114.29
8	O	700	ADP	PA-O3A-PB	-3.86	119.71	132.67
6	B	700	08T	PB-O3A-PA	-3.69	122.72	132.99
8	E	700	ADP	PA-O3A-PB	-3.56	120.72	132.67
6	M	700	08T	O4'-C1'-N9	-3.48	100.81	108.10
6	B	700	08T	O1A-PA-O2A	-3.46	108.38	118.70
6	M	700	08T	O1A-PA-O2A	-3.32	108.81	118.70
6	C	700	08T	O1A-PA-O2A	-3.31	108.84	118.70
6	D	700	08T	O1A-PA-O2A	-3.29	108.90	118.70
6	C	700	08T	O4'-C1'-N9	-3.04	101.73	108.10
8	E	700	ADP	C4-C5-N7	-2.80	106.90	109.48
6	D	700	08T	PB-O3A-PA	-2.77	125.26	132.99
6	L	700	08T	PB-O3A-PA	-2.74	125.36	132.99
6	N	700	08T	PB-O3A-PA	-2.56	125.85	132.99
6	L	700	08T	O2B-PB-O3A	-2.50	101.97	108.79
6	C	700	08T	O2B-PB-O1B	-2.37	111.64	118.70
6	N	700	08T	C5'-C4'-C3'	-2.35	105.87	115.21
8	O	700	ADP	C4-C5-N7	-2.32	107.35	109.48
6	L	700	08T	O2B-PB-O1B	-2.27	111.93	118.70
6	B	700	08T	C5'-C4'-C3'	-2.23	106.36	115.21
6	B	700	08T	O2B-PB-O1B	-2.08	112.50	118.70
6	M	700	08T	C2'-C3'-C4'	2.07	106.86	102.61
6	B	700	08T	C2'-C3'-C4'	2.10	106.93	102.61
6	C	700	08T	O3A-PB-O1B	2.19	114.03	108.79
6	C	700	08T	O5'-C5'-C4'	2.20	117.23	109.12
6	M	700	08T	O3A-PB-O3B	2.22	109.76	101.31
8	O	700	ADP	C2-N1-C6	2.25	122.79	118.77
6	L	700	08T	C4'-O4'-C1'	2.27	112.21	109.72
6	C	700	08T	C4'-O4'-C1'	2.29	112.24	109.72
6	B	700	08T	O3A-PB-O3B	2.36	110.27	101.31
8	O	700	ADP	O3B-PB-O2B	2.43	116.63	107.38
6	C	700	08T	C2'-C1'-N9	2.44	118.02	114.29
6	B	700	08T	O3A-PA-O2A	2.46	114.69	108.79
6	D	700	08T	O5'-C5'-C4'	2.47	118.22	109.12
6	D	700	08T	C4'-O4'-C1'	2.49	112.46	109.72
6	L	700	08T	C4-C5-N7	2.55	111.82	109.48
6	C	700	08T	O1A-PA-O3A	2.59	115.86	108.79
8	E	700	ADP	O3B-PB-O2B	2.74	117.81	107.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	700	08T	C4'-O4'-C1'	3.02	113.04	109.72
6	M	700	08T	O5'-C5'-C4'	3.11	120.60	109.12
6	C	700	08T	O3A-PB-O3B	3.12	113.18	101.31
6	L	700	08T	O3A-PB-O3B	3.47	114.51	101.31
6	M	700	08T	C4'-O4'-C1'	3.47	113.54	109.72
6	L	700	08T	O1A-PA-O3A	3.74	119.00	108.79

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 53 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	700	08T	8	0
6	C	700	08T	8	0
6	D	700	08T	6	0
8	E	700	ADP	5	0
6	L	700	08T	6	0
6	M	700	08T	9	0
6	N	700	08T	7	0
8	O	700	ADP	4	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	B	320/324 (98%)	-0.25	0 100 100	63, 76, 113, 193	0
1	C	320/324 (98%)	-0.27	2 (0%) 90 85	59, 69, 118, 169	0
1	D	320/324 (98%)	-0.31	0 100 100	58, 68, 132, 172	0
1	E	305/324 (94%)	-0.12	4 (1%) 79 70	64, 89, 143, 195	0
1	L	320/324 (98%)	-0.16	2 (0%) 90 85	68, 78, 141, 189	0
1	M	320/324 (98%)	-0.16	3 (0%) 85 78	60, 71, 139, 226	0
1	N	320/324 (98%)	-0.23	1 (0%) 94 91	58, 71, 134, 179	0
1	O	305/324 (94%)	-0.08	1 (0%) 94 91	64, 92, 144, 179	0
2	A	186/199 (93%)	0.15	2 (1%) 82 73	69, 102, 165, 217	0
2	K	186/199 (93%)	0.31	3 (1%) 74 65	78, 112, 163, 196	0
3	F	222/228 (97%)	0.16	2 (0%) 85 78	88, 112, 143, 182	0
3	G	222/228 (97%)	0.04	0 100 100	69, 90, 127, 157	0
3	H	222/228 (97%)	0.27	1 (0%) 91 88	73, 102, 144, 166	0
3	P	222/228 (97%)	0.22	3 (1%) 78 68	83, 112, 163, 221	0
3	Q	222/228 (97%)	-0.01	0 100 100	64, 87, 124, 153	0
3	R	222/228 (97%)	0.39	5 (2%) 64 54	62, 99, 147, 211	0
4	I	24/30 (80%)	-0.44	0 100 100	67, 94, 150, 160	0
4	S	24/30 (80%)	-0.21	0 100 100	66, 100, 164, 171	0
5	J	20/20 (100%)	-0.46	1 (5%) 32 25	66, 122, 185, 190	0
5	T	20/20 (100%)	-0.51	0 100 100	72, 104, 187, 196	0
All	All	4322/4458 (96%)	-0.05	30 (0%) 89 82	58, 89, 146, 226	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	0	SER	3.7
1	M	233	GLY	2.9
2	A	176	GLU	2.9
1	N	271	GLU	2.8
3	R	6211	GLY	2.8
1	M	319	LYS	2.7
1	C	319	LYS	2.7
3	P	7177	THR	2.5
3	P	7087	ARG	2.5
3	R	6068	ASN	2.4
1	O	9	HIS	2.4
5	J	20	DA	2.3
3	R	6213	HIS	2.3
2	A	168	LYS	2.2
1	L	245	LYS	2.2
1	C	239	LEU	2.2
2	K	60	TYR	2.2
2	K	37	GLU	2.1
3	R	6168	THR	2.1
1	E	319	LYS	2.1
1	E	220	LEU	2.1
3	R	6212	GLU	2.1
3	F	7181	ILE	2.1
3	F	7182	ILE	2.1
1	L	319	LYS	2.1
3	P	7142	VAL	2.1
2	K	36	ALA	2.0
1	E	187	ILE	2.0
1	E	201	PHE	2.0
3	H	6151	GLY	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
7	MG	N	800	1/1	0.97	0.34	4.66	65,65,65,65	0
7	MG	L	800	1/1	0.89	0.30	3.33	70,70,70,70	0
7	MG	M	800	1/1	0.84	0.33	2.92	63,63,63,63	0
7	MG	B	800	1/1	0.95	0.27	2.65	71,71,71,71	0
7	MG	D	800	1/1	0.97	0.29	2.14	63,63,63,63	0
7	MG	C	800	1/1	0.96	0.27	1.45	63,63,63,63	0
6	08T	L	700	31/31	0.97	0.22	-0.15	71,73,74,75	0
8	ADP	E	700	27/27	0.93	0.21	-0.35	80,85,87,88	0
8	ADP	O	700	27/27	0.93	0.22	-0.53	84,89,90,91	0
6	08T	M	700	31/31	0.96	0.20	-0.68	64,65,66,66	0
6	08T	D	700	31/31	0.97	0.20	-0.83	62,64,64,65	0
6	08T	C	700	31/31	0.97	0.20	-0.88	62,64,64,64	0
6	08T	B	700	31/31	0.97	0.20	-0.95	71,73,74,74	0
6	08T	N	700	31/31	0.96	0.20	-0.96	65,66,67,67	0
7	MG	O	801	1/1	0.91	0.58	-	83,83,83,83	0
7	MG	E	801	1/1	0.85	0.46	-	81,81,81,81	0

6.5 Other polymers

There are no such residues in this entry.