Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:25 AM GMT

PDB ID	:	2GXA
Title	:	Crystal structure of papillomavirus E1 hexameric helicase with ssDNA and MgADP
Authors	:	Enemark, E.J.; Joshua-Tor, L.
Deposited on	:	2006-05-08
Resolution	:	3.15 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:

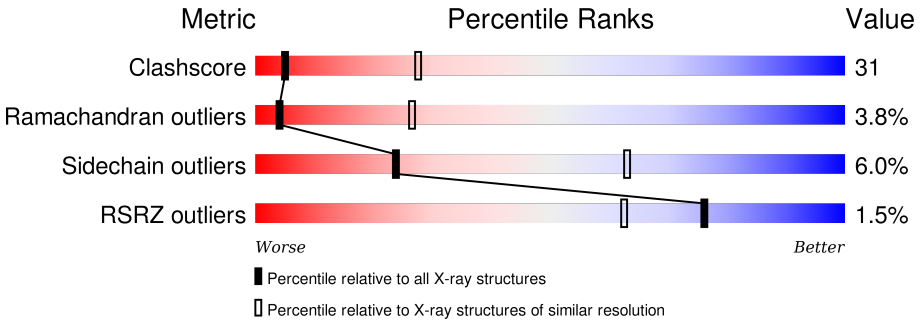
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.15 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))
Clashscore	102246	1249 (3.20-3.12)
Ramachandran outliers	100387	1222 (3.20-3.12)
Sidechain outliers	100360	1221 (3.20-3.12)
RSRZ outliers	91569	1117 (3.20-3.12)

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	M	13	8% 38% 54%
1	N	13	8% 38% 8% 46%
2	A	274	% 49% 44% 5% •
2	B	274	52% 41% 5% •
2	C	274	4% 60% 35% • •
2	D	274	% 49% 43% 6% •
2	E	274	53% 41% 6%

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Mol	Chain	Length	Quality of chain
2	F	274	48% 44% 5%
2	G	274	% 57% 38%
2	H	274	54% 42%
2	I	274	2% 49% 45% 5%
2	J	274	2% 51% 41% 6%
2	K	274	% 50% 44% 5%
2	L	274	5% 34% 52% 12%

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
3	MG	J	30	-	-	-	X
4	CL	B	42	-	-	X	-
5	ADP	F	6	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 26374 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 DNA chain called 5'-D(*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP *T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	M	6	Total	C	N	O	P	0	0	0
			121	60	12	43	6			
1	N	7	Total	C	N	O	P	0	0	0
			141	70	14	50	7			

- Molecule 2 is a protein called Replication protein E1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	270	Total	C	N	O	S	0	0	0
			2140	1380	371	379	10			
2	B	270	Total	C	N	O	S	0	0	0
			2140	1380	371	379	10			
2	C	270	Total	C	N	O	S	0	0	0
			2140	1380	371	379	10			
2	D	270	Total	C	N	O	S	0	0	0
			2140	1380	371	379	10			
2	E	274	Total	C	N	O	S	0	0	0
			2177	1402	377	388	10			
2	F	270	Total	C	N	O	S	0	0	0
			2140	1380	371	379	10			
2	G	270	Total	C	N	O	S	0	0	0
			2140	1380	371	379	10			
2	H	274	Total	C	N	O	S	0	0	0
			2177	1402	377	388	10			
2	I	270	Total	C	N	O	S	0	0	0
			2140	1380	371	379	10			
2	J	270	Total	C	N	O	S	0	0	0
			2140	1380	371	379	10			
2	K	273	Total	C	N	O	S	0	0	0
			2173	1400	376	387	10			
2	L	270	Total	C	N	O	S	0	0	0
			2140	1380	371	379	10			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	304	GLY	-	cloning artifact	UNP P03116
B	304	GLY	-	cloning artifact	UNP P03116
C	304	GLY	-	cloning artifact	UNP P03116
D	304	GLY	-	cloning artifact	UNP P03116
E	304	GLY	-	cloning artifact	UNP P03116
F	304	GLY	-	cloning artifact	UNP P03116
G	304	GLY	-	cloning artifact	UNP P03116
H	304	GLY	-	cloning artifact	UNP P03116
I	304	GLY	-	cloning artifact	UNP P03116
J	304	GLY	-	cloning artifact	UNP P03116
K	304	GLY	-	cloning artifact	UNP P03116
L	304	GLY	-	cloning artifact	UNP P03116

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	1	Total Mg 1 1	0	0
3	J	1	Total Mg 1 1	0	0
3	D	1	Total Mg 1 1	0	0
3	K	1	Total Mg 1 1	0	0
3	E	1	Total Mg 1 1	0	0
3	H	1	Total Mg 1 1	0	0
3	B	1	Total Mg 1 1	0	0
3	I	1	Total Mg 1 1	0	0
3	C	1	Total Mg 1 1	0	0
3	A	1	Total Mg 1 1	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	H	1	Total Cl 1 1	0	0

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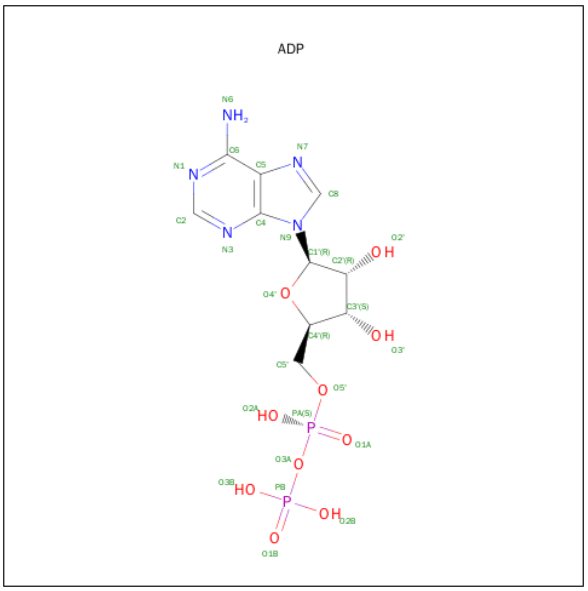
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Cl 1 1	0	0
4	A	1	Total Cl 1 1	0	0

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O P 27 10 5 10 2	0	0
5	B	1	Total C N O P 27 10 5 10 2	0	0
5	C	1	Total C N O P 27 10 5 10 2	0	0
5	D	1	Total C N O P 27 10 5 10 2	10	0
5	E	1	Total C N O P 27 10 5 10 2	10	0
5	F	1	Total C N O P 27 10 5 10 2	10	0
5	G	1	Total C N O P 27 10 5 10 2	0	0
5	H	1	Total C N O P 27 10 5 10 2	0	0
5	J	1	Total C N O P 27 10 5 10 2	10	0

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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	2	Total	O	0	0
			2	2		
6	B	3	Total	O	0	0
			3	3		
6	C	3	Total	O	0	0
			3	3		
6	D	1	Total	O	0	0
			1	1		
6	G	3	Total	O	0	0
			3	3		
6	H	2	Total	O	0	0
			2	2		
6	I	1	Total	O	0	0
			1	1		

3 Residue-property plots (i)

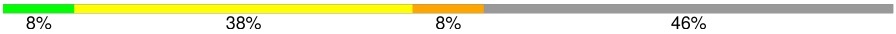
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: 5'-D(*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*T)-3'

Chain M:

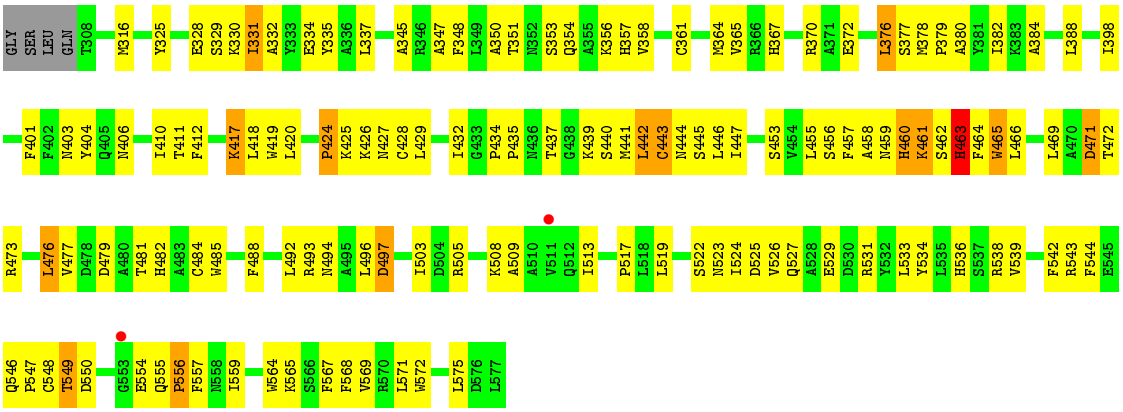
- Molecule 1: 5'-D(*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*T)-3'

Chain N:



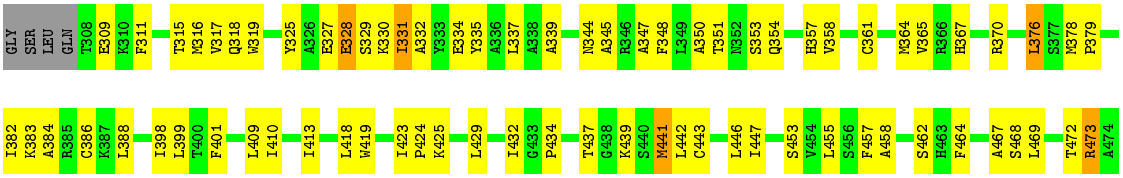
- Molecule 2: Replication protein E1

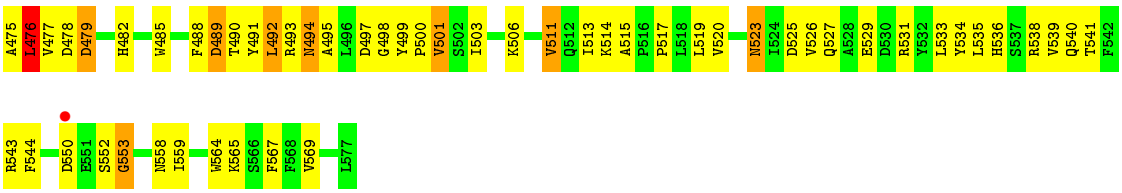
Chain A:



- Molecule 2: Replication protein E1

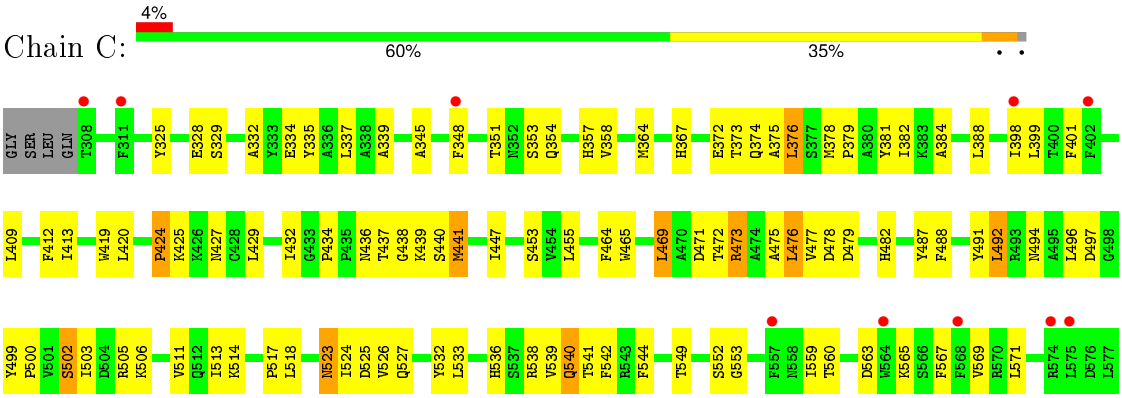
Chain B:





• Molecule 2: Replication protein E1

Chain C:

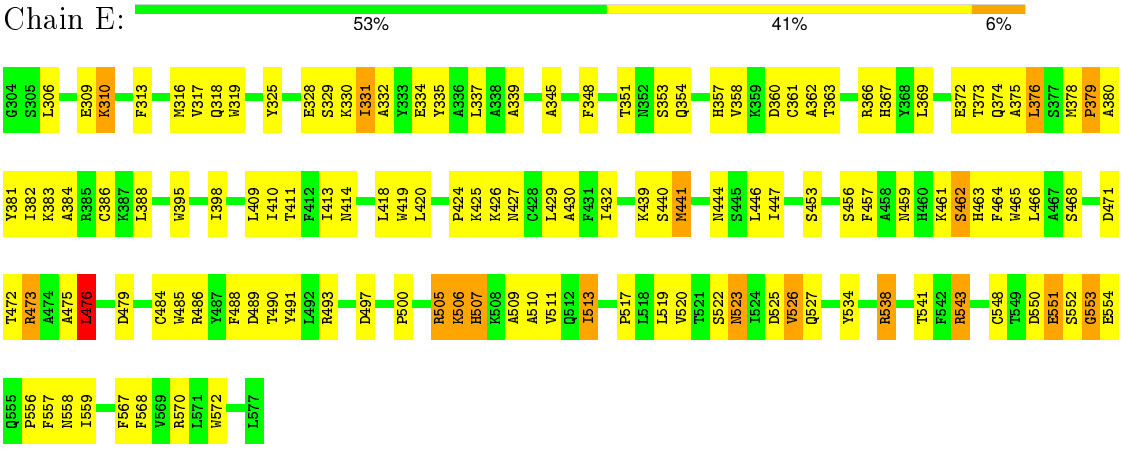


• Molecule 2: Replication protein E1

Chain D:

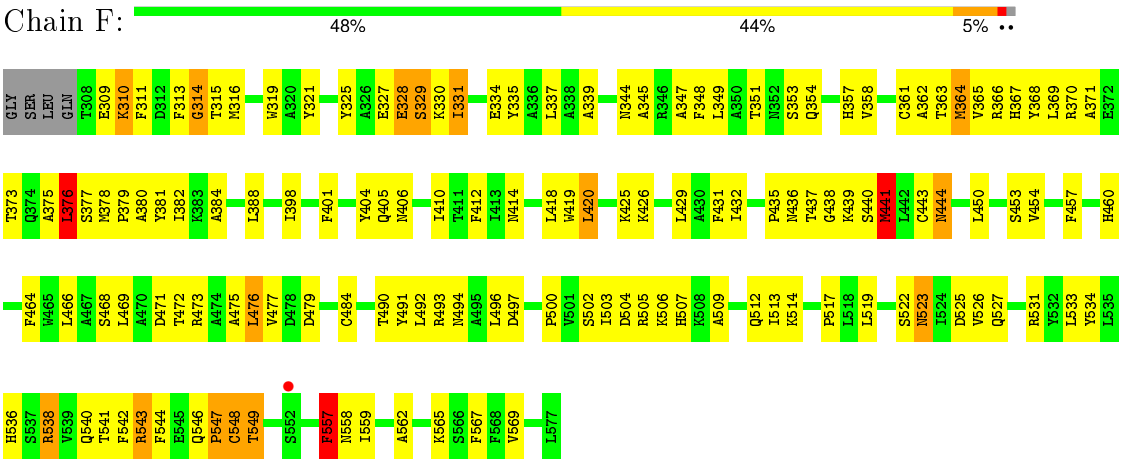
• Molecule 2: Replication protein E1

Chain E:



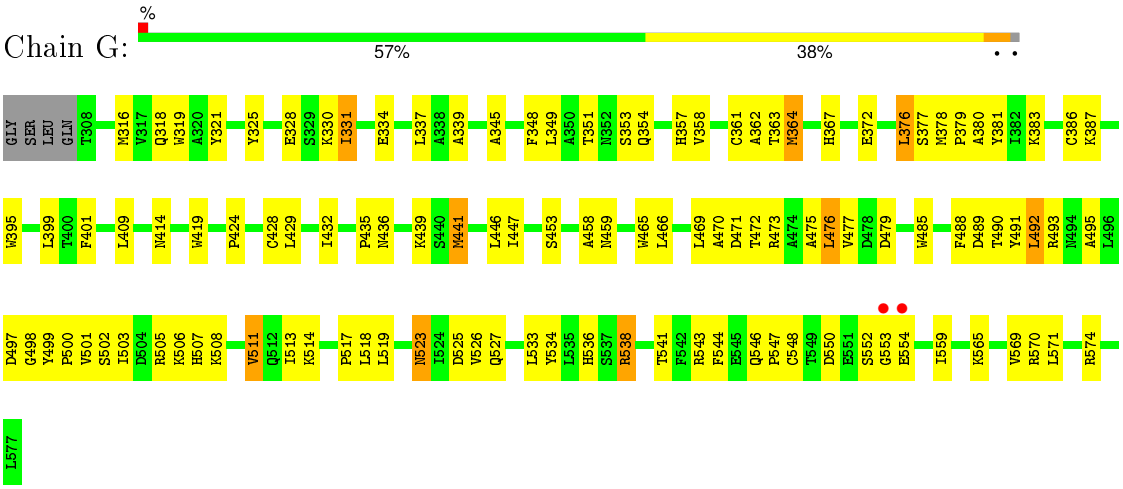
• Molecule 2: Replication protein E1

Chain F:



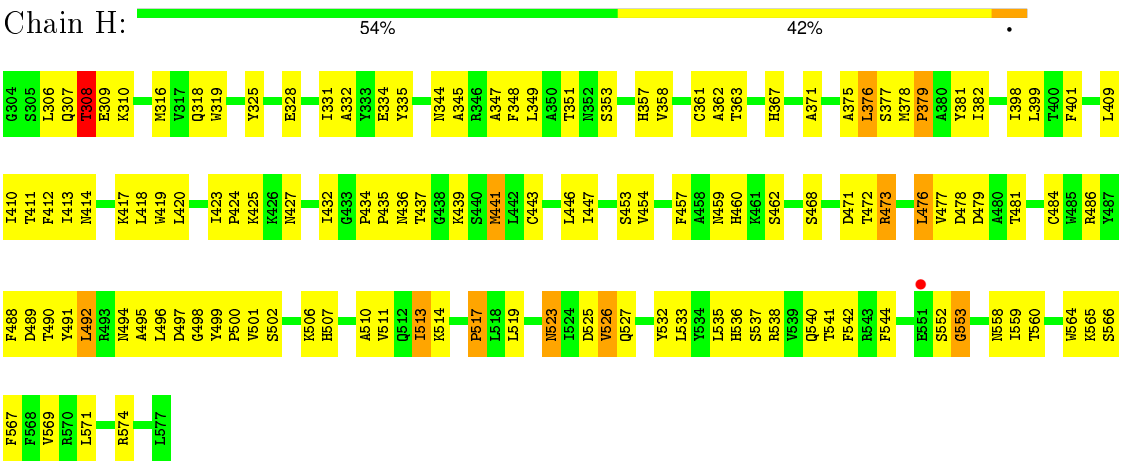
• Molecule 2: Replication protein E1

Chain G:



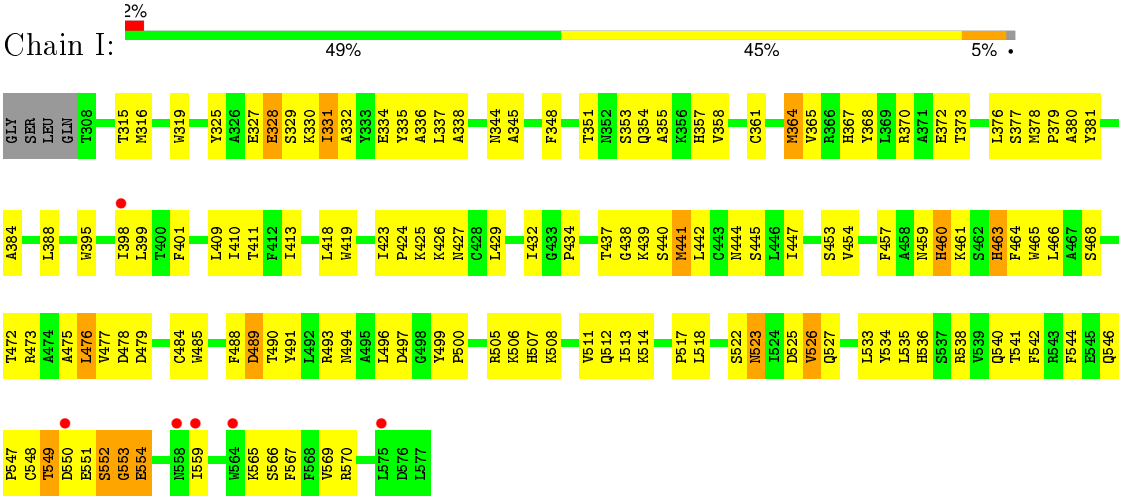
• Molecule 2: Replication protein E1

Chain H:



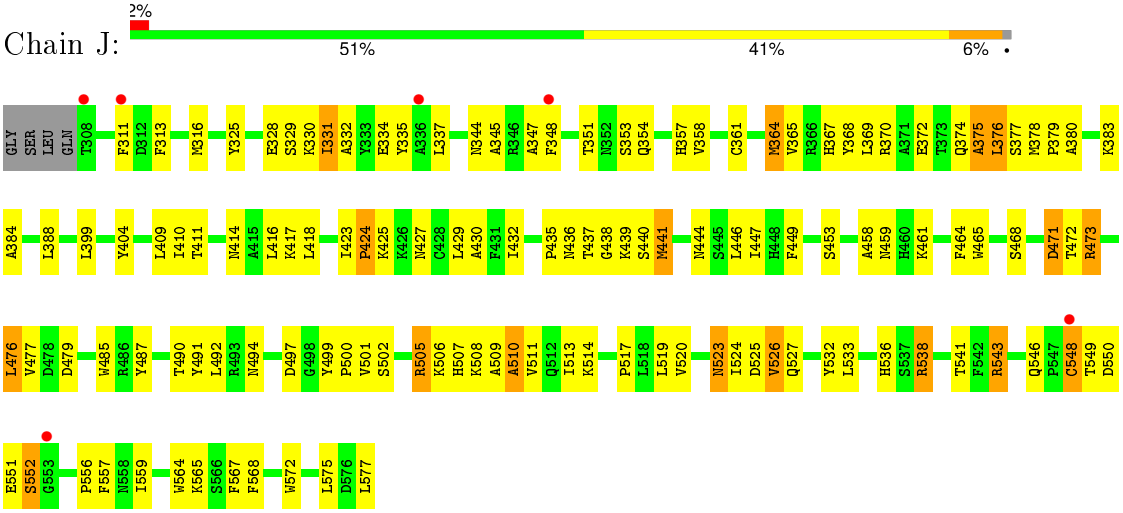
• Molecule 2: Replication protein E1

Chain I:



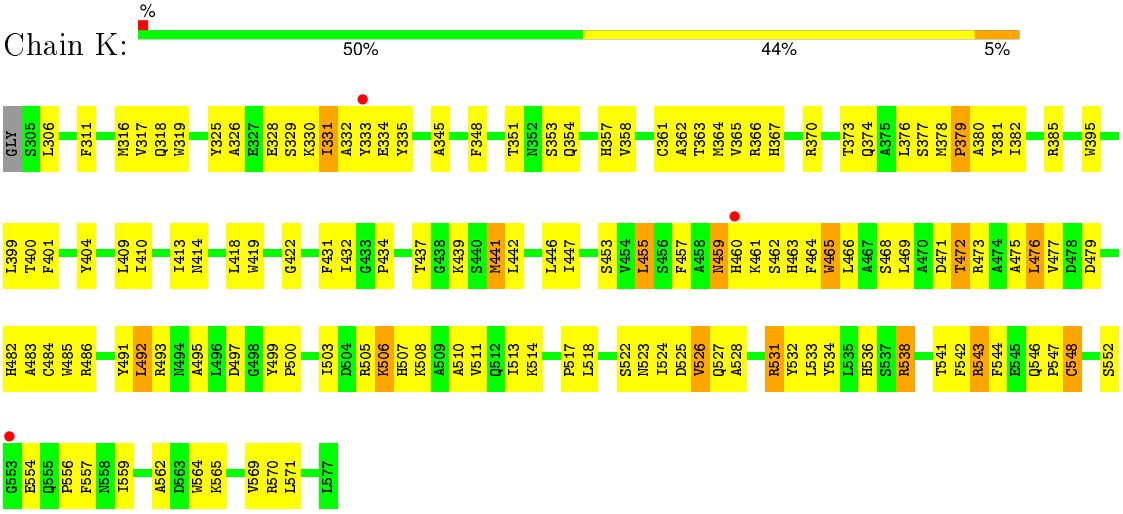
- Molecule 2: Replication protein E1

Chain J:



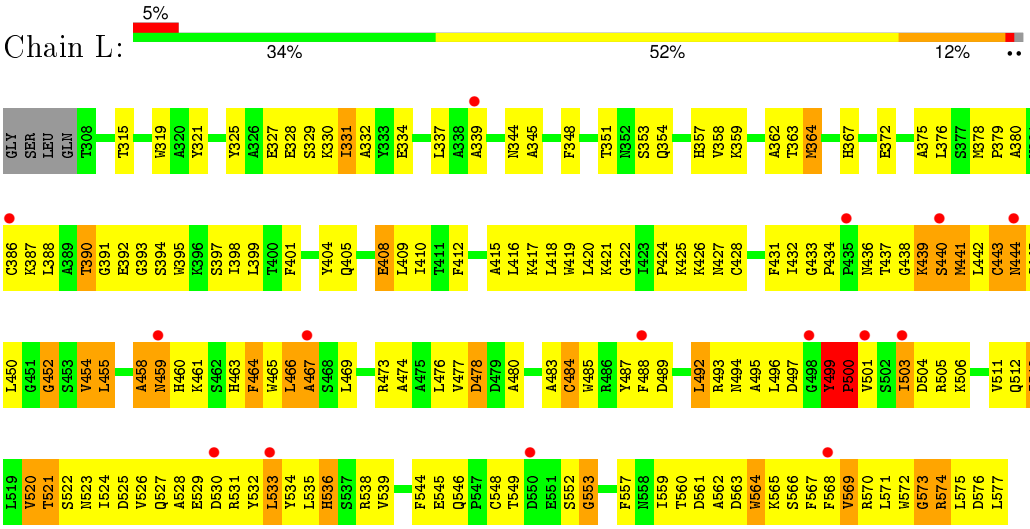
- Molecule 2: Replication protein E1

Chain K:



- Molecule 2: Replication protein E1

Chain L:


5%
34%
52%
12%
GLY SER LEU GLN T308 T315 W319 A320 Y321 Y326 A326 E327 E328 S329 K330 I331 A332 Y333 E334 L337 A338 A339 N344 A345 F348 T351 N352 S353 Q354 H357 V358 K359 A362 T363 M364 H367 E372 A375 L376 S377 M378 P379 A380 Y381 I382 K383 A384 R385
C386 K387 L388 A389 T390 G391 E392 G393 S394 W395 K396 S397 I398 L399 T400 F401 Y404 Q405 E408 L409 I410 T411 F412 A415 L416 K417 L418 W419 L420 K421 G422 I423 P424 K425 K426 N427 C428 F431 I432 G433 P434 P435 N436 T437 G438 K439 S440 M441 L442 C443 N444 S445 L446 I447 H448 F449
L450 G451 G452 S453 V454 L455 A458 N459 H460 K461 S462 H463 F464 W465 L466 A467 S468 L469 R473 A474 A475 L476 V477 D478 D479 A480 A483 C484 W485 R486 Y487 F488 D489 I492 R493 N494 A495 L496 D497 G498 Y499 P500 V501 S502 I503 D504 R505 K506 V511 Q512 I513 K514 P517 L518
L519 V520 T521 S522 N523 I524 D525 V526 Q527 A528 E529 D530 R531 Y532 L533 Y534 L535 H536 S537 R538 V539 F544 E545 Q546 P547 C548 T549 D550 E551 S552 G553 F557 N558 I559 T560 D561 A562 D563 W564 K565 S566 F567 F568 V569 R570 L571 W572 G573 R574 L575 D576 L577

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	100.51Å 100.88Å 125.02Å 92.60° 111.46° 106.01°	Depositor
Resolution (Å)	44.65 – 3.15 44.65 – 3.11	Depositor EDS
% Data completeness (in resolution range)	91.9 (44.65-3.15) 88.2 (44.65-3.11)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.33 (at 3.12Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.239 , 0.298 0.221 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	74.0	Xtriage
Anisotropy	0.151	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , 34.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 75699 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	26374	wwPDB-VP
Average B, all atoms (Å^2)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.23% 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, CL

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	M	0.83	1/132 (0.8%)	0.93	0/200
1	N	0.76	1/154 (0.6%)	0.82	0/234
2	A	0.71	4/2199 (0.2%)	0.89	6/2985 (0.2%)
2	B	0.48	0/2199	0.69	1/2985 (0.0%)
2	C	0.43	0/2199	0.62	0/2985
2	D	0.41	0/2199	0.61	0/2985
2	E	0.42	0/2236	0.64	2/3033 (0.1%)
2	F	0.42	0/2199	0.64	0/2985
2	G	0.43	0/2199	0.61	0/2985
2	H	0.44	0/2236	0.64	0/3033
2	I	0.41	0/2199	0.62	0/2985
2	J	0.42	0/2199	0.63	0/2985
2	K	0.44	0/2232	0.65	0/3028
2	L	0.39	0/2199	0.73	3/2985 (0.1%)
All	All	0.46	6/26781 (0.0%)	0.67	12/36393 (0.0%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	497	ASP	CB-CG	-10.66	1.29	1.51
2	A	484	CYS	CB-SG	-7.33	1.69	1.82
1	M	1	DT	OP3-P	-6.40	1.53	1.61
1	N	1	DT	OP3-P	-6.28	1.53	1.61
2	A	464	PHE	CB-CG	-5.80	1.41	1.51
2	A	460	HIS	CA-CB	-5.75	1.41	1.53

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	497	ASP	CB-CG-OD1	-15.82	104.06	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	L	500	PRO	CA-N-CD	-10.02	97.47	111.50
2	L	499	TYR	C-N-CD	-7.52	104.06	120.60
2	A	497	ASP	OD1-CG-OD2	7.47	137.50	123.30
2	E	476	LEU	CA-CB-CG	6.49	130.22	115.30
2	A	464	PHE	N-CA-C	-6.39	93.75	111.00
2	B	476	LEU	CA-CB-CG	6.34	129.89	115.30
2	A	442	LEU	CA-CB-CG	-6.29	100.84	115.30
2	L	499	TYR	N-CA-C	5.92	126.99	111.00
2	A	463	HIS	CB-CA-C	-5.84	98.73	110.40
2	A	443	CYS	CA-CB-SG	-5.25	104.55	114.00
2	E	558	ASN	N-CA-C	-5.05	97.36	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	M	121	0	73	15	0
1	N	141	0	85	19	0
2	A	2140	0	2078	161	0
2	B	2140	0	2078	127	0
2	C	2140	0	2078	92	0
2	D	2140	0	2078	122	0
2	E	2177	0	2124	113	0
2	F	2140	0	2078	134	0
2	G	2140	0	2078	99	0
2	H	2177	0	2125	127	0
2	I	2140	0	2077	132	0
2	J	2140	0	2078	118	0
2	K	2173	0	2121	139	0
2	L	2140	0	2078	279	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
3	K	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	2	0
4	H	1	0	0	0	0
5	A	27	0	12	4	0
5	B	27	0	12	5	0
5	C	27	0	12	4	0
5	D	27	0	12	2	0
5	E	27	0	12	2	0
5	F	27	0	12	11	0
5	G	27	0	12	3	0
5	H	27	0	12	5	0
5	J	27	0	12	1	0
5	K	27	0	12	1	0
5	L	27	0	12	3	0
6	A	2	0	0	0	0
6	B	3	0	0	0	0
6	C	3	0	0	0	0
6	D	1	0	0	0	0
6	G	3	0	0	0	0
6	H	2	0	0	0	0
6	I	1	0	0	0	0
All	All	26374	0	25361	1595	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 31.

All (1595) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:534:TYR:HE2	2:A:538:ARG:NH1	1.19	1.34
2:A:534:TYR:CE2	2:A:538:ARG:NH1	1.95	1.33
2:L:444:ASN:HD21	2:L:521:THR:HG21	1.05	1.15
2:L:505:ARG:HH21	2:L:511:VAL:HB	1.08	1.10
2:L:512:GLN:O	2:L:513:ILE:HG13	1.51	1.10
2:L:444:ASN:ND2	2:L:521:THR:CG2	2.15	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:513:ILE:HG22	2:L:514:LYS:H	1.09	1.08
2:L:444:ASN:ND2	2:L:521:THR:HG21	1.72	1.02
2:L:497:ASP:O	2:L:499:TYR:CD2	2.14	1.01
5:B:2:ADP:O2A	2:C:425:LYS:HD2	1.62	1.00
2:C:432:ILE:HD13	2:C:525:ASP:HA	1.40	1.00
2:H:432:ILE:HD13	2:H:525:ASP:HA	1.41	1.00
2:L:513:ILE:HG22	2:L:514:LYS:N	1.73	1.00
2:L:390:THR:HG21	2:L:561:ASP:HB2	1.43	0.99
2:L:442:LEU:O	2:L:446:LEU:HG	1.62	0.98
2:A:534:TYR:HE2	2:A:538:ARG:HH12	1.02	0.98
2:L:513:ILE:CG2	2:L:514:LYS:H	1.75	0.98
2:A:534:TYR:CE2	2:A:538:ARG:CZ	2.47	0.97
2:I:432:ILE:HD13	2:I:525:ASP:HA	1.45	0.97
2:J:351:THR:HG22	2:J:353:SER:H	1.29	0.96
2:F:376:LEU:H	2:F:376:LEU:CD2	1.79	0.96
2:L:431:PHE:HD1	2:L:440:SER:HG	0.97	0.96
2:K:455:LEU:HD23	2:K:455:LEU:N	1.80	0.95
2:L:444:ASN:HD22	2:L:521:THR:HG22	1.31	0.94
2:A:455:LEU:C	2:A:465:TRP:HZ3	1.71	0.94
2:B:453:SER:HB3	2:B:472:THR:HG21	1.50	0.94
2:B:493:ARG:HD3	2:B:538:ARG:HH12	1.31	0.93
2:L:444:ASN:ND2	2:L:521:THR:HG22	1.83	0.93
2:I:325:TYR:CE1	2:I:334:GLU:HG2	2.05	0.92
2:L:418:LEU:HD12	2:L:418:LEU:H	1.33	0.92
2:A:424:PRO:O	2:A:425:LYS:HG2	1.67	0.92
2:A:328:GLU:HB3	2:B:367:HIS:HE1	1.33	0.92
2:E:453:SER:HB3	2:E:472:THR:HG21	1.50	0.92
2:L:489:ASP:HB2	2:L:535:LEU:HD11	1.50	0.92
2:L:454:VAL:HG12	2:L:455:LEU:H	1.35	0.91
2:A:534:TYR:OH	2:A:538:ARG:NH2	2.03	0.91
2:L:446:LEU:CD1	2:L:559:ILE:HB	1.99	0.91
2:C:539:VAL:HG12	2:C:540:GLN:O	1.71	0.91
2:F:376:LEU:H	2:F:376:LEU:HD22	1.35	0.91
2:K:441:MET:HE3	2:K:559:ILE:H	1.34	0.90
2:B:432:ILE:HD13	2:B:525:ASP:HA	1.53	0.90
2:L:325:TYR:CE1	2:L:334:GLU:HG2	2.07	0.90
2:A:418:LEU:H	2:A:418:LEU:HD12	1.36	0.90
2:A:432:ILE:HD13	2:A:525:ASP:HA	1.53	0.90
2:J:494:ASN:OD1	2:J:499:TYR:HB2	1.72	0.90
2:L:440:SER:HB2	2:L:443:CYS:HB2	1.55	0.89
2:D:513:ILE:HD12	2:D:514:LYS:H	1.36	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:442:LEU:O	2:L:446:LEU:CG	2.20	0.89
2:L:454:VAL:O	2:L:455:LEU:HG	1.72	0.89
2:L:434:PRO:HD2	2:L:544:PHE:O	1.73	0.88
2:L:447:ILE:HG12	2:L:564:TRP:CE2	2.08	0.88
2:L:444:ASN:HD21	2:L:521:THR:CG2	1.78	0.88
2:G:533:LEU:HA	2:G:536:HIS:CE1	2.09	0.88
2:L:505:ARG:NH2	2:L:511:VAL:HB	1.89	0.88
2:H:489:ASP:HA	2:H:535:LEU:HD21	1.55	0.88
2:A:455:LEU:HB3	2:A:465:TRP:CZ3	2.08	0.88
1:M:3:DT:H5'	2:D:507:HIS:CD2	2.10	0.87
2:J:432:ILE:HD13	2:J:525:ASP:HA	1.55	0.87
2:L:497:ASP:O	2:L:499:TYR:HD2	1.55	0.87
2:D:533:LEU:HA	2:D:536:HIS:CE1	2.10	0.87
2:L:454:VAL:HG12	2:L:455:LEU:N	1.86	0.87
2:E:427:ASN:HD21	2:E:517:PRO:HA	1.38	0.87
2:E:427:ASN:ND2	2:E:517:PRO:HA	1.90	0.86
2:L:351:THR:HG22	2:L:353:SER:H	1.39	0.86
2:D:351:THR:HG22	2:D:353:SER:H	1.40	0.86
2:K:432:ILE:HD13	2:K:525:ASP:HA	1.57	0.86
2:L:461:LYS:HE3	2:L:487:TYR:HD1	1.40	0.86
2:D:432:ILE:HD13	2:D:525:ASP:HA	1.57	0.85
2:F:473:ARG:O	2:F:517:PRO:HD2	1.77	0.85
2:F:432:ILE:HD13	2:F:525:ASP:HA	1.57	0.85
2:K:455:LEU:HD21	2:K:475:ALA:HB1	1.57	0.84
1:M:3:DT:H1'	1:M:4:DT:H5"	1.58	0.84
2:A:351:THR:HG22	2:A:353:SER:H	1.42	0.84
2:L:454:VAL:CG1	2:L:455:LEU:H	1.91	0.84
2:H:439:LYS:HE3	5:H:8:ADP:O2B	1.78	0.84
2:G:439:LYS:HE3	5:G:7:ADP:O2B	1.78	0.83
2:A:441:MET:HG3	2:A:442:LEU:N	1.92	0.83
2:I:439:LYS:HE3	5:J:9:ADP:O2B	1.79	0.82
2:C:351:THR:HG22	2:C:353:SER:H	1.41	0.82
2:C:453:SER:HB3	2:C:472:THR:HG21	1.61	0.82
2:D:399:LEU:HD13	2:D:409:LEU:HD22	1.62	0.81
2:B:494:ASN:HD22	2:B:494:ASN:H	1.27	0.81
2:D:439:LYS:HE3	5:D:4:ADP:O2B	1.81	0.81
2:K:328:GLU:HB3	2:L:367:HIS:HE1	1.44	0.81
2:K:306:LEU:H	2:K:306:LEU:HD22	1.45	0.81
2:C:376:LEU:HD23	2:C:381:TYR:HA	1.61	0.81
2:J:453:SER:HB3	2:J:472:THR:HG21	1.60	0.81
2:L:494:ASN:O	2:L:499:TYR:HB3	1.81	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:538:ARG:HG3	2:L:539:VAL:HG23	1.63	0.81
2:A:328:GLU:HB3	2:B:367:HIS:CE1	2.15	0.80
2:B:523:ASN:HD22	2:B:523:ASN:N	1.79	0.80
2:F:351:THR:HG22	2:F:353:SER:H	1.46	0.80
2:L:511:VAL:HG22	2:L:512:GLN:H	1.46	0.80
2:B:351:THR:HG22	2:B:353:SER:H	1.47	0.80
2:L:446:LEU:HB3	2:L:564:TRP:HZ3	1.47	0.79
2:A:459:ASN:O	2:A:465:TRP:HB2	1.81	0.79
2:B:527:GLN:NE2	2:B:539:VAL:O	2.15	0.79
2:I:376:LEU:HD12	2:I:380:ALA:HB1	1.62	0.79
2:L:438:GLY:O	2:L:440:SER:N	2.16	0.79
2:C:488:PHE:CE1	2:C:492:LEU:HD23	2.17	0.79
2:B:493:ARG:HD3	2:B:538:ARG:NH1	1.97	0.79
2:H:351:THR:HG22	2:H:353:SER:H	1.46	0.79
2:D:500:PRO:HA	2:D:514:LYS:HA	1.65	0.79
2:H:453:SER:HB3	2:H:472:THR:HG21	1.65	0.79
2:H:523:ASN:N	2:H:523:ASN:HD22	1.81	0.79
2:L:476:LEU:HD13	2:L:477:VAL:N	1.98	0.79
2:F:441:MET:HB2	5:F:6:ADP:O4'	1.81	0.79
2:A:455:LEU:C	2:A:465:TRP:CZ3	2.56	0.79
2:I:325:TYR:HE1	2:I:334:GLU:HG2	1.48	0.78
2:C:439:LYS:HE3	5:C:3:ADP:O2B	1.82	0.78
2:E:376:LEU:HD12	2:E:380:ALA:HB1	1.65	0.78
2:F:373:THR:O	2:F:376:LEU:HD23	1.83	0.78
2:A:476:LEU:HD22	2:A:477:VAL:N	1.97	0.78
2:E:439:LYS:HE3	5:E:5:ADP:O2B	1.82	0.78
2:J:378:MET:HB3	2:J:379:PRO:HD3	1.65	0.78
2:L:442:LEU:O	2:L:446:LEU:CD1	2.31	0.77
2:K:459:ASN:O	2:K:461:LYS:N	2.17	0.77
2:L:379:PRO:HB3	2:L:577:LEU:HD22	1.66	0.77
2:L:485:TRP:CE3	2:L:526:VAL:HG11	2.19	0.77
2:A:441:MET:CG	2:A:442:LEU:N	2.47	0.77
2:G:325:TYR:CE1	2:G:334:GLU:HG2	2.19	0.77
2:F:410:ILE:HG12	2:F:414:ASN:ND2	1.99	0.77
2:L:445:SER:O	2:L:446:LEU:HD23	1.85	0.77
2:D:325:TYR:CE1	2:D:334:GLU:HG2	2.18	0.77
2:D:395:TRP:CD1	2:D:396:LYS:N	2.53	0.77
2:J:473:ARG:O	2:J:517:PRO:HD2	1.85	0.77
2:H:325:TYR:CE1	2:H:334:GLU:HG2	2.20	0.77
2:B:531:ARG:HD3	2:K:486:ARG:HH21	1.50	0.77
2:L:446:LEU:HD13	2:L:559:ILE:HB	1.64	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:432:ILE:HD13	2:G:525:ASP:HA	1.65	0.76
2:J:439:LYS:HE3	5:K:10:ADP:O2B	1.85	0.76
2:I:523:ASN:N	2:I:523:ASN:HD22	1.80	0.76
2:D:523:ASN:HD22	2:D:523:ASN:N	1.82	0.76
2:D:395:TRP:HD1	2:D:396:LYS:H	1.33	0.76
2:L:434:PRO:HG2	2:L:437:THR:OG1	1.86	0.76
2:B:325:TYR:CE1	2:B:334:GLU:HG2	2.19	0.76
2:G:399:LEU:HD13	2:G:409:LEU:HD22	1.68	0.75
2:F:376:LEU:HD22	2:F:376:LEU:N	2.02	0.75
2:H:376:LEU:HD23	2:H:381:TYR:HA	1.67	0.75
2:E:325:TYR:CE1	2:E:334:GLU:HG2	2.21	0.75
2:A:534:TYR:CZ	2:A:538:ARG:NH2	2.53	0.75
2:A:460:HIS:HA	2:A:465:TRP:HB3	1.69	0.74
2:J:325:TYR:CE1	2:J:334:GLU:HG2	2.23	0.74
2:A:456:SER:N	2:A:465:TRP:HZ3	1.86	0.74
2:E:432:ILE:HD13	2:E:525:ASP:HA	1.69	0.74
2:I:464:PHE:CD2	2:I:506:LYS:HG2	2.23	0.74
2:K:351:THR:HG22	2:K:353:SER:H	1.53	0.74
2:F:438:GLY:HA2	5:F:6:ADP:H4'	1.69	0.74
2:F:437:THR:OG1	2:F:439:LYS:HE2	1.88	0.74
2:C:523:ASN:HD22	2:C:523:ASN:N	1.85	0.73
2:L:533:LEU:HA	2:L:536:HIS:CE1	2.23	0.73
2:K:377:SER:OG	2:K:379:PRO:HD2	1.88	0.73
2:E:523:ASN:N	2:E:523:ASN:HD22	1.86	0.73
2:F:364:MET:O	2:F:367:HIS:HB2	1.88	0.73
2:I:424:PRO:HA	2:I:497:ASP:O	1.89	0.73
2:I:464:PHE:CE2	2:I:506:LYS:HG2	2.24	0.73
2:L:460:HIS:NE2	2:L:463:HIS:HB2	2.03	0.73
2:H:378:MET:HE2	2:H:473:ARG:HH12	1.54	0.73
2:B:473:ARG:O	2:B:517:PRO:HD2	1.87	0.73
2:K:373:THR:HA	2:K:376:LEU:CD2	2.19	0.72
2:L:432:ILE:HD13	2:L:525:ASP:HA	1.69	0.72
1:N:3:DT:H1'	1:N:4:DT:H5"	1.70	0.72
2:H:488:PHE:CD1	2:H:496:LEU:HD21	2.25	0.72
2:L:476:LEU:HD22	2:L:477:VAL:H	1.52	0.72
2:J:505:ARG:NH1	2:J:505:ARG:HB2	2.05	0.72
2:L:434:PRO:HD2	2:L:437:THR:HG21	1.70	0.72
2:L:444:ASN:OD1	2:L:445:SER:N	2.23	0.72
2:H:476:LEU:HD22	2:H:477:VAL:N	2.05	0.72
2:L:494:ASN:HB2	2:L:501:VAL:HG22	1.70	0.72
2:I:427:ASN:ND2	2:I:517:PRO:HA	2.04	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:523:ASN:N	2:J:523:ASN:HD22	1.87	0.72
2:F:441:MET:SD	2:F:559:ILE:HG12	2.30	0.71
2:B:370:ARG:HH11	2:B:370:ARG:HG2	1.55	0.71
2:L:447:ILE:CG1	2:L:564:TRP:CZ2	2.74	0.71
2:B:494:ASN:HD22	2:B:494:ASN:N	1.88	0.71
2:B:418:LEU:HD12	2:B:418:LEU:N	2.04	0.71
2:B:439:LYS:HE3	5:B:2:ADP:O2B	1.91	0.71
2:H:425:LYS:HG2	2:H:497:ASP:OD1	1.89	0.71
2:E:485:TRP:CE3	2:E:526:VAL:HG11	2.26	0.71
2:L:390:THR:HG21	2:L:561:ASP:CB	2.21	0.71
2:F:377:SER:H	2:F:380:ALA:HB3	1.56	0.71
2:G:493:ARG:HD3	2:G:534:TYR:CE2	2.26	0.71
2:K:373:THR:HA	2:K:376:LEU:HD23	1.72	0.70
2:L:437:THR:HG21	2:L:545:GLU:HA	1.70	0.70
2:E:486:ARG:HD3	2:L:528:ALA:O	1.90	0.70
1:M:3:DT:H5'	2:D:507:HIS:HD2	1.56	0.70
2:E:453:SER:CB	2:E:472:THR:HG21	2.19	0.70
2:A:460:HIS:NE2	2:A:461:LYS:HE2	2.07	0.70
2:B:354:GLN:O	2:B:358:VAL:HG23	1.92	0.70
2:I:453:SER:HB3	2:I:472:THR:HG21	1.74	0.70
2:K:455:LEU:HD23	2:K:455:LEU:H	1.52	0.70
2:G:533:LEU:HA	2:G:536:HIS:ND1	2.06	0.70
2:L:485:TRP:CD2	2:L:526:VAL:HG11	2.27	0.70
2:L:496:LEU:HD13	2:L:538:ARG:HD2	1.73	0.70
2:E:486:ARG:HE	2:L:528:ALA:HA	1.56	0.70
2:L:399:LEU:HD13	2:L:409:LEU:HD22	1.73	0.70
2:C:432:ILE:CD1	2:C:525:ASP:HA	2.21	0.69
2:A:455:LEU:CB	2:A:465:TRP:CZ3	2.74	0.69
2:I:345:ALA:O	2:I:348:PHE:HB3	1.91	0.69
2:H:432:ILE:CD1	2:H:525:ASP:HA	2.21	0.69
1:N:1:DT:H72	1:N:2:DT:H3	1.56	0.69
2:A:534:TYR:CZ	2:A:538:ARG:CZ	2.74	0.69
2:L:418:LEU:HD22	2:L:426:LYS:HD2	1.74	0.69
2:C:401:PHE:HE2	2:C:544:PHE:HE2	1.40	0.69
2:J:550:ASP:CB	2:J:556:PRO:HD3	2.22	0.69
2:L:512:GLN:O	2:L:513:ILE:CG1	2.34	0.69
2:B:453:SER:CB	2:B:472:THR:HG21	2.22	0.69
2:B:478:ASP:HB3	2:C:494:ASN:HD21	1.58	0.69
2:D:441:MET:HE1	2:D:559:ILE:HB	1.73	0.69
2:B:499:TYR:HB3	2:B:500:PRO:HD2	1.74	0.69
2:A:325:TYR:CE1	2:A:334:GLU:HG2	2.27	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:372:GLU:O	2:J:376:LEU:HD22	1.92	0.69
2:L:390:THR:HG22	2:L:562:ALA:HB2	1.75	0.69
2:L:452:GLY:HA3	2:L:474:ALA:O	1.93	0.69
2:A:460:HIS:CD2	2:A:461:LYS:HD3	2.28	0.69
2:D:530:ASP:CG	2:G:533:LEU:HD21	2.14	0.68
2:J:476:LEU:HD22	2:J:477:VAL:N	2.07	0.68
2:A:459:ASN:O	2:A:465:TRP:CB	2.41	0.68
2:E:525:ASP:OD1	2:E:527:GLN:HB2	1.93	0.68
2:L:419:TRP:NE1	2:L:518:LEU:O	2.27	0.68
2:L:418:LEU:HD22	2:L:426:LYS:CD	2.24	0.68
2:L:421:LYS:NZ	2:L:576:ASP:HB3	2.08	0.68
2:A:523:ASN:ND2	2:B:534:TYR:CE1	2.62	0.68
2:D:489:ASP:HA	2:D:535:LEU:HD21	1.75	0.68
2:L:398:ILE:HG22	2:L:399:LEU:N	2.06	0.68
2:A:401:PHE:HE2	2:A:544:PHE:CE2	2.11	0.68
2:A:456:SER:N	2:A:465:TRP:CZ3	2.61	0.68
2:A:418:LEU:CD1	2:A:418:LEU:H	2.06	0.68
2:D:424:PRO:HA	2:D:497:ASP:O	1.94	0.68
2:I:368:TYR:O	2:I:372:GLU:HB2	1.93	0.68
2:F:440:SER:O	2:F:444:ASN:HB2	1.93	0.68
2:E:351:THR:HG22	2:E:353:SER:H	1.58	0.68
2:L:532:TYR:HB3	2:L:535:LEU:HD13	1.76	0.68
2:D:395:TRP:HD1	2:D:396:LYS:N	1.91	0.67
2:L:442:LEU:O	2:L:446:LEU:HD12	1.95	0.67
2:L:533:LEU:HD23	2:L:533:LEU:H	1.59	0.67
2:E:372:GLU:O	2:E:375:ALA:HB3	1.95	0.67
2:F:418:LEU:N	2:F:418:LEU:HD12	2.09	0.67
2:G:453:SER:HB3	2:G:472:THR:HG21	1.76	0.67
2:F:436:ASN:HA	5:F:6:ADP:O2A	1.95	0.67
2:H:377:SER:OG	2:H:379:PRO:HD2	1.94	0.67
2:F:438:GLY:O	2:F:441:MET:HB3	1.94	0.67
2:D:526:VAL:HG12	2:D:532:TYR:CD1	2.30	0.67
2:A:382:ILE:HD11	2:A:420:LEU:HD22	1.75	0.67
2:B:441:MET:HE3	2:B:558:ASN:HA	1.76	0.67
2:C:476:LEU:HD22	2:C:477:VAL:N	2.10	0.67
2:C:436:ASN:HD21	2:C:549:THR:CB	2.08	0.67
2:F:325:TYR:CE1	2:F:334:GLU:HG2	2.29	0.66
2:E:376:LEU:HD12	2:E:380:ALA:CB	2.25	0.66
2:J:377:SER:H	2:J:380:ALA:HB3	1.59	0.66
2:G:419:TRP:CE2	2:G:517:PRO:HB3	2.31	0.66
2:B:332:ALA:HB2	2:B:358:VAL:HG11	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:328:GLU:HB3	2:K:367:HIS:HE1	1.60	0.66
2:F:476:LEU:HD22	2:F:477:VAL:N	2.10	0.66
2:L:325:TYR:HE1	2:L:334:GLU:HG2	1.60	0.66
2:D:427:ASN:OD1	2:D:517:PRO:HA	1.95	0.66
2:K:328:GLU:HB3	2:L:367:HIS:CE1	2.29	0.66
2:A:361:CYS:O	2:A:365:VAL:HG23	1.95	0.66
2:L:466:LEU:HG	2:L:467:ALA:N	2.10	0.66
2:A:531:ARG:HH22	2:K:527:GLN:C	1.99	0.66
2:L:483:ALA:C	2:L:485:TRP:H	1.99	0.66
2:H:376:LEU:HD23	2:H:381:TYR:CA	2.26	0.66
2:C:401:PHE:HE2	2:C:544:PHE:CE2	2.14	0.66
2:G:552:SER:O	2:G:554:GLU:N	2.29	0.66
2:A:457:PHE:N	2:A:465:TRP:CZ3	2.63	0.65
2:A:440:SER:O	2:A:444:ASN:HB2	1.95	0.65
2:B:490:THR:HG22	2:B:491:TYR:CD2	2.31	0.65
2:I:513:ILE:HG13	2:I:514:LYS:H	1.61	0.65
2:H:533:LEU:HA	2:H:536:HIS:CE1	2.31	0.65
1:N:3:DT:H1'	2:J:507:HIS:HE1	1.61	0.65
2:F:513:ILE:HG13	2:F:514:LYS:N	2.12	0.65
2:A:403:ASN:O	2:A:406:ASN:N	2.29	0.65
2:L:446:LEU:HB3	2:L:564:TRP:CZ3	2.31	0.65
2:A:453:SER:HB3	2:A:472:THR:HG21	1.78	0.65
2:L:437:THR:O	2:L:437:THR:HG22	1.96	0.65
2:K:325:TYR:CE1	2:K:334:GLU:HG2	2.32	0.65
2:D:460:HIS:HA	2:D:465:TRP:CD1	2.32	0.65
2:L:401:PHE:O	2:L:404:TYR:HB3	1.97	0.64
2:L:505:ARG:HE	2:L:511:VAL:CG1	2.09	0.64
2:D:523:ASN:ND2	2:D:523:ASN:N	2.45	0.64
2:H:447:ILE:HG13	2:H:476:LEU:HB2	1.79	0.64
5:G:7:ADP:O2A	2:H:425:LYS:HD2	1.98	0.64
2:H:382:ILE:HD11	2:H:420:LEU:HD22	1.78	0.64
2:G:354:GLN:O	2:G:358:VAL:HG23	1.97	0.64
2:L:512:GLN:C	2:L:513:ILE:HG13	2.18	0.64
2:F:513:ILE:HG13	2:F:514:LYS:H	1.61	0.64
2:K:378:MET:O	2:K:382:ILE:HG13	1.97	0.64
2:C:332:ALA:HB2	2:C:358:VAL:HG11	1.77	0.64
2:D:476:LEU:HD22	2:D:477:VAL:N	2.13	0.64
2:G:523:ASN:HD22	2:G:523:ASN:N	1.95	0.64
2:I:513:ILE:CG1	2:I:514:LYS:H	2.10	0.64
2:I:525:ASP:OD1	2:I:527:GLN:HB2	1.98	0.64
2:F:453:SER:HB3	2:F:472:THR:HG21	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:419:TRP:CD1	2:C:429:LEU:HG	2.33	0.64
2:E:446:LEU:HD23	2:E:519:LEU:HD11	1.79	0.64
2:B:455:LEU:HD21	2:B:469:LEU:HD21	1.79	0.64
2:J:364:MET:O	2:J:367:HIS:HB2	1.98	0.64
2:L:372:GLU:O	2:L:376:LEU:HD23	1.98	0.63
2:L:480:ALA:HB1	2:L:484:CYS:HB3	1.80	0.63
2:A:439:LYS:HE3	5:A:1:ADP:O2B	1.99	0.63
2:C:399:LEU:HD13	2:C:409:LEU:HD22	1.81	0.63
2:A:548:CYS:O	2:A:550:ASP:N	2.31	0.63
2:K:419:TRP:O	2:K:422:GLY:N	2.24	0.63
2:A:466:LEU:O	2:A:503:ILE:HD12	1.99	0.63
2:I:447:ILE:HG13	2:I:476:LEU:HB2	1.79	0.63
2:J:376:LEU:H	2:J:376:LEU:HD22	1.62	0.63
2:A:497:ASP:N	2:A:497:ASP:OD1	2.28	0.62
2:C:447:ILE:HG13	2:C:476:LEU:HB2	1.81	0.62
2:A:378:MET:HB3	2:A:379:PRO:HD3	1.81	0.62
2:A:418:LEU:N	2:A:418:LEU:HD12	2.10	0.62
2:G:490:THR:HG22	2:G:491:TYR:CD2	2.35	0.62
2:L:434:PRO:CG	2:L:437:THR:OG1	2.48	0.62
2:H:489:ASP:CA	2:H:535:LEU:HD21	2.28	0.62
2:K:499:TYR:HB3	2:K:500:PRO:HD2	1.79	0.62
2:B:376:LEU:N	2:B:376:LEU:HD12	2.14	0.62
2:K:453:SER:CB	2:K:472:THR:HG21	2.30	0.62
2:J:432:ILE:HD12	2:J:541:THR:HG21	1.81	0.62
2:B:376:LEU:H	2:B:376:LEU:HD12	1.63	0.62
2:I:332:ALA:HB2	2:I:358:VAL:HG11	1.81	0.62
2:G:447:ILE:HG13	2:G:476:LEU:HB2	1.80	0.62
2:G:503:ILE:O	2:G:511:VAL:HG23	2.00	0.62
2:L:390:THR:CG2	2:L:561:ASP:HB2	2.24	0.62
2:F:469:LEU:HB2	2:F:503:ILE:HD13	1.80	0.62
2:D:328:GLU:HB3	2:E:367:HIS:CE1	2.35	0.62
2:J:505:ARG:HH11	2:J:505:ARG:HB2	1.63	0.62
2:A:367:HIS:CE1	2:F:328:GLU:HB3	2.34	0.62
1:M:3:DT:C1'	1:M:4:DT:H5"	2.30	0.62
2:H:424:PRO:HA	2:H:497:ASP:O	2.00	0.62
2:F:401:PHE:O	2:F:404:TYR:HB3	2.00	0.62
2:H:501:VAL:HG22	2:H:502:SER:N	2.15	0.62
2:C:439:LYS:HB2	5:C:3:ADP:O2B	1.99	0.62
2:D:534:TYR:O	2:D:538:ARG:NH1	2.33	0.62
2:K:459:ASN:HB2	2:K:465:TRP:HB3	1.80	0.62
2:I:485:TRP:CE3	2:I:526:VAL:HG11	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:523:ASN:HD22	2:F:523:ASN:N	1.97	0.62
2:L:434:PRO:CD	2:L:544:PHE:O	2.47	0.61
2:I:513:ILE:HG13	2:I:514:LYS:N	2.15	0.61
2:C:559:ILE:HG22	2:C:560:THR:N	2.14	0.61
2:K:455:LEU:CD2	2:K:455:LEU:N	2.55	0.61
2:B:424:PRO:HA	2:B:497:ASP:O	2.00	0.61
2:H:441:MET:HE3	2:H:559:ILE:H	1.64	0.61
2:L:438:GLY:HA2	2:L:441:MET:SD	2.39	0.61
2:E:384:ALA:O	2:E:388:LEU:HD23	1.99	0.61
2:J:458:ALA:HB2	2:K:491:TYR:HB3	1.80	0.61
2:H:439:LYS:HB2	5:H:8:ADP:O2B	2.01	0.61
2:K:513:ILE:HG13	2:K:514:LYS:N	2.15	0.61
2:L:446:LEU:C	2:L:448:HIS:H	2.01	0.61
1:N:3:DT:H3'	2:I:464:PHE:HE2	1.65	0.61
2:G:330:LYS:O	2:G:331:ILE:C	2.37	0.61
2:I:533:LEU:HA	2:I:536:HIS:CE1	2.36	0.61
2:B:401:PHE:HE2	2:B:544:PHE:CE2	2.19	0.61
2:L:447:ILE:HG12	2:L:564:TRP:CZ2	2.34	0.61
2:B:364:MET:O	2:B:367:HIS:HB2	2.00	0.61
2:A:419:TRP:CE2	2:A:517:PRO:HB3	2.35	0.61
2:B:347:ALA:O	2:B:350:ALA:HB3	2.00	0.61
2:K:419:TRP:CE2	2:K:517:PRO:HB3	2.36	0.61
2:A:364:MET:O	2:A:367:HIS:HB2	2.01	0.61
2:F:497:ASP:OD2	2:F:538:ARG:NH1	2.33	0.61
2:E:378:MET:HB3	2:E:379:PRO:HD3	1.82	0.61
2:J:351:THR:HG22	2:J:353:SER:N	2.10	0.60
2:J:372:GLU:O	2:J:376:LEU:CD2	2.48	0.60
2:D:435:PRO:O	2:D:436:ASN:HB2	2.01	0.60
2:A:465:TRP:O	2:A:465:TRP:CG	2.53	0.60
2:J:399:LEU:HD13	2:J:409:LEU:HD22	1.83	0.60
2:L:447:ILE:HG13	2:L:564:TRP:CZ2	2.36	0.60
2:L:418:LEU:HD12	2:L:418:LEU:N	2.11	0.60
2:F:419:TRP:CE2	2:F:517:PRO:HB3	2.36	0.60
2:I:398:ILE:HD12	2:I:567:PHE:HB2	1.82	0.60
2:B:376:LEU:H	2:B:376:LEU:CD1	2.15	0.60
2:G:476:LEU:HD22	2:G:477:VAL:N	2.16	0.60
2:G:351:THR:HG22	2:G:353:SER:H	1.65	0.60
2:I:457:PHE:CZ	2:I:484:CYS:HA	2.36	0.60
5:A:1:ADP:O2A	2:B:425:LYS:HD2	2.02	0.60
2:D:565:LYS:O	2:D:569:VAL:HG23	2.00	0.60
2:F:354:GLN:O	2:F:358:VAL:HG23	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:533:LEU:HA	2:K:536:HIS:CE1	2.37	0.60
2:L:421:LYS:HZ1	2:L:576:ASP:HB3	1.66	0.60
2:D:513:ILE:HD12	2:D:514:LYS:N	2.13	0.60
2:H:523:ASN:N	2:H:523:ASN:ND2	2.46	0.60
2:C:345:ALA:O	2:C:348:PHE:HB3	2.02	0.60
2:G:376:LEU:HD23	2:G:381:TYR:HA	1.82	0.60
2:G:525:ASP:OD1	2:G:527:GLN:HB2	2.00	0.60
2:L:493:ARG:HH21	2:L:534:TYR:HD1	1.50	0.60
2:B:488:PHE:CE1	2:B:492:LEU:HD23	2.36	0.60
2:C:494:ASN:O	2:C:497:ASP:HB2	2.02	0.59
2:E:306:LEU:HD13	2:E:306:LEU:O	2.01	0.59
2:C:525:ASP:OD1	2:C:527:GLN:HB2	2.02	0.59
2:E:486:ARG:HD2	2:L:530:ASP:OD2	2.01	0.59
2:I:384:ALA:O	2:I:388:LEU:HD23	2.02	0.59
2:I:438:GLY:O	2:I:441:MET:HB3	2.02	0.59
2:C:401:PHE:CE2	2:C:544:PHE:CE2	2.91	0.59
2:I:351:THR:HG22	2:I:353:SER:H	1.67	0.59
2:K:464:PHE:C	2:K:466:LEU:H	2.05	0.59
2:H:488:PHE:CE1	2:H:492:LEU:HD23	2.36	0.59
2:B:335:TYR:CE2	2:B:345:ALA:HA	2.37	0.59
2:A:465:TRP:O	2:A:466:LEU:HD23	2.02	0.59
2:B:354:GLN:OE1	2:C:364:MET:HG2	2.03	0.59
2:I:453:SER:O	2:I:475:ALA:HA	2.02	0.59
2:F:345:ALA:O	2:F:348:PHE:HB3	2.02	0.59
2:K:565:LYS:O	2:K:569:VAL:HG23	2.01	0.59
2:B:523:ASN:N	2:B:523:ASN:ND2	2.46	0.59
2:F:418:LEU:H	2:F:418:LEU:HD12	1.65	0.59
2:E:378:MET:O	2:E:382:ILE:HG13	2.03	0.59
2:A:354:GLN:O	2:A:358:VAL:HG23	2.03	0.59
2:E:505:ARG:NH1	2:E:509:ALA:O	2.33	0.59
2:L:494:ASN:O	2:L:496:LEU:N	2.30	0.59
2:L:477:VAL:HB	2:L:520:VAL:HG13	1.84	0.59
2:H:378:MET:HE2	2:H:473:ARG:NH1	2.17	0.59
2:E:523:ASN:N	2:E:523:ASN:ND2	2.50	0.59
2:B:446:LEU:HD23	2:B:519:LEU:HD11	1.84	0.59
2:L:488:PHE:HB3	2:L:538:ARG:NH2	2.18	0.59
2:D:432:ILE:HG23	2:D:522:SER:O	2.03	0.59
2:D:348:PHE:CZ	2:D:354:GLN:HB3	2.38	0.59
2:A:429:LEU:HB2	2:A:519:LEU:HD23	1.84	0.58
2:D:349:LEU:HA	2:D:354:GLN:HE21	1.67	0.58
2:D:376:LEU:HD12	2:D:380:ALA:HB1	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:466:LEU:HG	2:L:467:ALA:H	1.66	0.58
2:H:525:ASP:OD1	2:H:527:GLN:HB2	2.03	0.58
2:A:529:GLU:HG2	2:A:531:ARG:HE	1.68	0.58
2:H:526:VAL:HG12	2:H:532:TYR:CD1	2.37	0.58
2:L:467:ALA:C	2:L:469:LEU:H	2.06	0.58
2:I:354:GLN:O	2:I:358:VAL:HG23	2.04	0.58
2:C:325:TYR:CE1	2:C:334:GLU:HG2	2.38	0.58
2:F:464:PHE:CD1	2:F:506:LYS:HD2	2.38	0.58
2:J:548:CYS:O	2:J:548:CYS:SG	2.61	0.58
2:J:505:ARG:NH1	2:J:509:ALA:O	2.30	0.58
2:L:448:HIS:ND1	2:L:449:PHE:N	2.51	0.58
5:H:8:ADP:H5'1	2:I:425:LYS:HD2	1.86	0.58
2:D:395:TRP:CE2	2:D:570:ARG:NH1	2.72	0.58
2:D:453:SER:N	2:D:472:THR:HG21	2.19	0.58
2:K:485:TRP:CE3	2:K:526:VAL:HG11	2.38	0.58
2:C:523:ASN:ND2	2:C:523:ASN:N	2.52	0.58
2:J:328:GLU:HB3	2:K:367:HIS:CE1	2.39	0.58
2:L:440:SER:O	2:L:444:ASN:OD1	2.22	0.58
2:L:436:ASN:C	2:L:438:GLY:H	2.05	0.58
2:L:446:LEU:HA	2:L:448:HIS:ND1	2.18	0.58
2:B:439:LYS:HB2	5:B:2:ADP:O2B	2.03	0.58
2:E:548:CYS:SG	2:E:557:PHE:HD1	2.27	0.58
2:L:385:ARG:HA	2:L:388:LEU:HD23	1.86	0.58
2:D:316:MET:CE	2:D:361:CYS:HB2	2.33	0.58
2:K:523:ASN:N	2:K:523:ASN:HD22	2.01	0.58
2:D:330:LYS:O	2:D:331:ILE:C	2.41	0.58
2:K:476:LEU:C	2:K:476:LEU:HD22	2.24	0.58
2:A:432:ILE:CD1	2:A:525:ASP:HA	2.32	0.58
2:J:525:ASP:OD2	2:J:543:ARG:NH1	2.36	0.58
2:K:459:ASN:HB2	2:K:465:TRP:CB	2.33	0.58
2:G:453:SER:N	2:G:472:THR:HG21	2.19	0.58
2:L:434:PRO:HD3	2:L:545:GLU:CD	2.24	0.57
2:B:500:PRO:HA	2:B:514:LYS:HA	1.85	0.57
2:A:367:HIS:HE1	2:F:328:GLU:HB3	1.68	0.57
2:I:500:PRO:HA	2:I:514:LYS:HA	1.86	0.57
2:I:548:CYS:O	2:I:549:THR:C	2.41	0.57
2:D:531:ARG:HH12	2:L:524:ILE:HG12	1.69	0.57
2:L:565:LYS:O	2:L:569:VAL:HG23	2.05	0.57
2:K:462:SER:C	2:K:464:PHE:H	2.07	0.57
2:A:447:ILE:HG13	2:A:476:LEU:HB2	1.86	0.57
2:H:376:LEU:HD23	2:H:381:TYR:N	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:476:LEU:HD22	2:C:476:LEU:C	2.25	0.57
2:I:513:ILE:CG1	2:I:514:LYS:N	2.67	0.57
2:G:513:ILE:HD12	2:G:514:LYS:H	1.68	0.57
2:I:489:ASP:HA	2:I:535:LEU:HD21	1.86	0.57
2:G:331:ILE:HD13	2:G:361:CYS:SG	2.43	0.57
2:J:438:GLY:O	2:J:441:MET:HB3	2.04	0.57
2:E:427:ASN:HD21	2:E:517:PRO:CA	2.13	0.57
2:E:395:TRP:NE1	2:E:570:ARG:HD3	2.19	0.57
2:L:467:ALA:C	2:L:469:LEU:N	2.55	0.57
2:E:465:TRP:NE1	2:E:466:LEU:HG	2.20	0.57
2:L:492:LEU:HD11	2:L:501:VAL:HG11	1.86	0.57
2:D:425:LYS:HG2	2:D:497:ASP:OD1	2.05	0.57
2:C:478:ASP:OD2	2:D:494:ASN:ND2	2.37	0.57
2:C:384:ALA:O	2:C:388:LEU:HD23	2.04	0.57
2:L:461:LYS:HE3	2:L:487:TYR:CD1	2.31	0.57
2:F:432:ILE:HD12	2:F:541:THR:HG21	1.87	0.57
2:J:523:ASN:N	2:J:523:ASN:ND2	2.52	0.57
2:G:364:MET:HE1	2:L:332:ALA:HB1	1.87	0.57
2:G:476:LEU:HD22	2:G:476:LEU:C	2.26	0.56
2:K:469:LEU:HB2	2:K:503:ILE:HD13	1.87	0.56
2:G:458:ALA:HB2	2:H:491:TYR:HB3	1.86	0.56
2:L:433:GLY:O	2:L:523:ASN:HA	2.05	0.56
2:I:330:LYS:O	2:I:331:ILE:C	2.44	0.56
2:L:505:ARG:HE	2:L:511:VAL:HG12	1.69	0.56
2:L:511:VAL:HG22	2:L:512:GLN:N	2.18	0.56
5:B:2:ADP:H5'1	2:C:425:LYS:HD2	1.87	0.56
2:C:464:PHE:CE2	2:C:506:LYS:HG2	2.40	0.56
2:H:494:ASN:O	2:H:497:ASP:HB2	2.05	0.56
1:N:2:DT:H2"	1:N:3:DT:C6	2.41	0.56
2:L:458:ALA:O	2:L:460:HIS:N	2.39	0.56
2:H:488:PHE:CE1	2:H:496:LEU:HD21	2.40	0.56
2:E:486:ARG:NE	2:L:528:ALA:HA	2.21	0.56
2:F:523:ASN:ND2	2:F:523:ASN:N	2.54	0.56
2:F:531:ARG:HH22	2:K:404:TYR:HD1	1.53	0.56
2:E:345:ALA:O	2:E:348:PHE:HB3	2.05	0.56
2:L:439:LYS:O	2:L:439:LYS:HG3	2.05	0.56
2:B:503:ILE:O	2:B:511:VAL:HG23	2.05	0.56
2:I:418:LEU:HD23	2:I:426:LYS:HD3	1.86	0.56
2:H:453:SER:HB3	2:H:472:THR:CG2	2.32	0.56
2:G:379:PRO:O	2:G:383:LYS:HB2	2.06	0.56
2:A:554:GLU:O	2:A:556:PRO:HD3	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:446:LEU:HA	2:L:448:HIS:CE1	2.40	0.56
2:L:446:LEU:CA	2:L:448:HIS:ND1	2.69	0.56
2:E:382:ILE:HD11	2:E:420:LEU:HD22	1.86	0.56
2:L:418:LEU:H	2:L:418:LEU:CD1	2.10	0.56
2:A:446:LEU:HD13	2:A:564:TRP:CH2	2.41	0.56
2:G:345:ALA:O	2:G:348:PHE:HB3	2.05	0.56
2:I:476:LEU:HD22	2:I:477:VAL:N	2.21	0.56
2:A:533:LEU:HA	2:A:536:HIS:CE1	2.40	0.56
2:B:485:TRP:CD2	2:B:526:VAL:HG11	2.40	0.56
2:C:412:PHE:HA	2:C:542:PHE:HZ	1.70	0.56
2:H:494:ASN:HD22	2:H:494:ASN:N	2.02	0.56
2:J:379:PRO:O	2:J:383:LYS:HB2	2.05	0.56
2:A:345:ALA:O	2:A:348:PHE:HB3	2.06	0.56
2:I:410:ILE:HG23	2:I:411:THR:N	2.21	0.56
2:L:566:SER:HA	2:L:569:VAL:HB	1.88	0.56
2:A:456:SER:C	2:A:465:TRP:CZ3	2.79	0.56
2:A:332:ALA:HB2	2:A:358:VAL:HG11	1.86	0.56
2:F:363:THR:HG22	2:F:367:HIS:CD2	2.40	0.56
2:I:473:ARG:O	2:I:517:PRO:HD2	2.05	0.56
2:H:478:ASP:HB3	2:I:494:ASN:HD21	1.70	0.56
2:B:418:LEU:N	2:B:418:LEU:CD1	2.69	0.56
2:B:424:PRO:O	2:B:425:LYS:HB2	2.04	0.55
1:N:1:DT:H2"	1:N:2:DT:C6	2.41	0.55
2:J:430:ALA:HA	2:J:520:VAL:O	2.05	0.55
2:E:453:SER:HB3	2:E:472:THR:CG2	2.30	0.55
2:D:395:TRP:CD1	2:D:396:LYS:HG3	2.41	0.55
2:J:476:LEU:HD22	2:J:476:LEU:C	2.26	0.55
2:E:485:TRP:CD2	2:E:526:VAL:HG11	2.40	0.55
2:E:330:LYS:O	2:E:331:ILE:C	2.43	0.55
2:L:446:LEU:CD1	2:L:559:ILE:CB	2.80	0.55
2:L:382:ILE:O	2:L:386:CYS:SG	2.57	0.55
2:E:335:TYR:CE2	2:E:345:ALA:HA	2.40	0.55
2:B:489:ASP:HA	2:B:535:LEU:HD21	1.89	0.55
2:K:453:SER:N	2:K:472:THR:HG21	2.21	0.55
2:F:315:THR:HB	2:F:344:ASN:ND2	2.20	0.55
2:L:431:PHE:HD1	2:L:440:SER:OG	1.77	0.55
2:L:562:ALA:O	2:L:565:LYS:HB3	2.06	0.55
2:B:525:ASP:OD1	2:B:527:GLN:HB2	2.06	0.55
2:L:485:TRP:CZ3	2:L:526:VAL:HG21	2.42	0.55
2:G:377:SER:H	2:G:380:ALA:HB3	1.72	0.55
2:H:410:ILE:HG23	2:H:411:THR:N	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:418:LEU:HD12	2:H:418:LEU:N	2.22	0.55
2:A:428:CYS:SG	2:A:539:VAL:HG13	2.45	0.55
2:D:496:LEU:HD23	2:D:518:LEU:HD12	1.89	0.55
2:F:376:LEU:HB3	2:F:380:ALA:HB3	1.88	0.55
1:M:4:DT:H4'	2:E:507:HIS:CE1	2.42	0.55
2:D:351:THR:HG21	2:D:357:HIS:CD2	2.41	0.55
2:I:328:GLU:O	2:I:329:SER:C	2.43	0.55
2:H:332:ALA:HB1	2:I:364:MET:HE3	1.88	0.55
2:H:565:LYS:O	2:H:569:VAL:HG23	2.07	0.55
2:A:461:LYS:C	2:A:463:HIS:H	2.10	0.55
2:I:361:CYS:O	2:I:365:VAL:HG23	2.08	0.55
2:C:373:THR:O	2:C:375:ALA:N	2.40	0.55
2:H:319:TRP:HH2	2:H:334:GLU:HB3	1.72	0.55
1:N:3:DT:H1'	2:J:507:HIS:CE1	2.41	0.55
2:K:473:ARG:O	2:K:517:PRO:HD2	2.07	0.55
2:L:383:LYS:HG3	2:L:384:ALA:N	2.22	0.54
2:L:569:VAL:HG12	2:L:570:ARG:N	2.21	0.54
2:D:473:ARG:O	2:D:517:PRO:HD2	2.07	0.54
2:G:328:GLU:HB3	2:H:367:HIS:CE1	2.42	0.54
2:L:562:ALA:O	2:L:565:LYS:N	2.40	0.54
2:J:427:ASN:ND2	2:J:517:PRO:HA	2.22	0.54
2:C:335:TYR:CE2	2:C:345:ALA:HA	2.42	0.54
2:C:434:PRO:O	2:C:437:THR:HG23	2.07	0.54
2:H:432:ILE:HD12	2:H:541:THR:HG21	1.89	0.54
2:H:453:SER:CB	2:H:472:THR:HG21	2.36	0.54
2:K:330:LYS:O	2:K:331:ILE:C	2.45	0.54
2:D:453:SER:HB3	2:D:472:THR:HG21	1.90	0.54
2:J:441:MET:C	2:J:441:MET:SD	2.85	0.54
2:I:432:ILE:HA	2:I:522:SER:O	2.07	0.54
2:J:453:SER:HB3	2:J:472:THR:CG2	2.36	0.54
2:H:478:ASP:HB3	2:I:494:ASN:ND2	2.22	0.54
2:K:447:ILE:HG13	2:K:476:LEU:HB2	1.90	0.54
2:E:465:TRP:CD1	2:E:466:LEU:HG	2.42	0.54
2:G:328:GLU:HB3	2:H:367:HIS:HE1	1.72	0.54
2:F:378:MET:HB3	2:F:379:PRO:HD3	1.88	0.54
1:M:4:DT:C4'	2:E:507:HIS:HE1	2.20	0.54
2:D:399:LEU:O	2:D:400:THR:C	2.45	0.54
2:J:446:LEU:HD23	2:J:519:LEU:HD11	1.87	0.54
2:D:332:ALA:HB2	2:D:358:VAL:HG11	1.89	0.54
2:E:507:HIS:CE1	2:F:507:HIS:HD2	2.26	0.54
2:L:446:LEU:CB	2:L:564:TRP:CZ3	2.91	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:446:LEU:C	2:L:448:HIS:N	2.61	0.54
2:B:439:LYS:NZ	4:B:42:CL:CL	2.78	0.54
2:A:523:ASN:ND2	2:B:534:TYR:CZ	2.76	0.54
2:L:461:LYS:NZ	2:L:483:ALA:HB1	2.23	0.54
2:K:404:TYR:CE2	2:K:546:GLN:HB3	2.43	0.54
2:D:328:GLU:HB3	2:E:367:HIS:HE1	1.72	0.54
2:H:559:ILE:HG22	2:H:560:THR:N	2.23	0.54
2:H:335:TYR:CE2	2:H:345:ALA:HA	2.43	0.54
2:F:565:LYS:O	2:F:569:VAL:HG23	2.07	0.54
2:L:438:GLY:HA3	2:L:548:CYS:HB2	1.90	0.54
2:F:382:ILE:HD11	2:F:420:LEU:HD22	1.89	0.54
2:K:381:TYR:O	2:K:385:ARG:HG2	2.08	0.54
2:L:440:SER:CB	2:L:443:CYS:HB2	2.35	0.54
2:L:505:ARG:HH21	2:L:511:VAL:CB	2.00	0.54
2:L:494:ASN:C	2:L:496:LEU:H	2.11	0.54
2:L:380:ALA:O	2:L:383:LYS:HG2	2.08	0.54
2:A:476:LEU:C	2:A:476:LEU:HD22	2.28	0.54
2:J:465:TRP:HZ2	2:J:487:TYR:CE2	2.26	0.54
2:L:546:GLN:N	2:L:546:GLN:OE1	2.42	0.53
2:A:503:ILE:O	2:A:503:ILE:HG22	2.07	0.53
2:B:348:PHE:CZ	2:B:354:GLN:HB3	2.43	0.53
2:G:513:ILE:HG13	2:G:514:LYS:N	2.23	0.53
2:B:529:GLU:HG2	2:B:531:ARG:HE	1.72	0.53
2:G:453:SER:CB	2:G:472:THR:HG21	2.38	0.53
2:G:505:ARG:CZ	2:G:511:VAL:HG21	2.38	0.53
2:A:330:LYS:O	2:A:331:ILE:C	2.47	0.53
2:D:363:THR:HA	2:D:366:ARG:HD2	1.89	0.53
2:I:523:ASN:N	2:I:523:ASN:ND2	2.48	0.53
2:J:358:VAL:HG21	2:K:364:MET:CE	2.38	0.53
2:F:548:CYS:SG	2:F:549:THR:N	2.82	0.53
2:L:559:ILE:HG22	2:L:560:THR:O	2.08	0.53
2:K:455:LEU:HD13	2:K:466:LEU:HD23	1.91	0.53
2:B:453:SER:HB3	2:B:472:THR:CG2	2.32	0.53
2:H:453:SER:N	2:H:472:THR:HG21	2.23	0.53
2:H:307:GLN:O	2:H:308:THR:O	2.25	0.53
2:F:476:LEU:HD22	2:F:476:LEU:C	2.28	0.53
2:K:335:TYR:CE2	2:K:345:ALA:HA	2.43	0.53
2:L:467:ALA:O	2:L:503:ILE:HG13	2.08	0.53
2:C:505:ARG:CZ	2:C:511:VAL:CG2	2.87	0.53
2:B:565:LYS:O	2:B:569:VAL:HG23	2.09	0.53
2:L:401:PHE:HZ	2:L:405:GLN:HE21	1.56	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:441:MET:HB2	5:F:6:ADP:C1'	2.38	0.53
2:A:335:TYR:CE2	2:A:345:ALA:HA	2.43	0.53
2:F:344:ASN:O	2:F:347:ALA:HB3	2.08	0.53
2:L:434:PRO:HG2	2:L:437:THR:HG21	1.91	0.53
2:F:525:ASP:OD1	2:F:527:GLN:HB2	2.08	0.53
2:K:378:MET:N	2:K:379:PRO:CD	2.71	0.53
2:H:501:VAL:HG22	2:H:502:SER:H	1.71	0.53
2:D:377:SER:H	2:D:380:ALA:HB3	1.74	0.53
2:F:547:PRO:O	2:F:548:CYS:HB3	2.09	0.53
2:H:506:LYS:O	2:H:507:HIS:HB2	2.07	0.53
1:M:2:DT:H3'	2:C:464:PHE:HE2	1.74	0.53
2:E:409:LEU:O	2:E:413:ILE:HG13	2.09	0.53
2:A:446:LEU:HD23	2:A:519:LEU:HD11	1.91	0.53
2:E:430:ALA:HA	2:E:520:VAL:O	2.08	0.53
2:L:489:ASP:CB	2:L:535:LEU:HD11	2.33	0.52
2:K:453:SER:O	2:K:475:ALA:HA	2.10	0.52
1:N:3:DT:H2"	1:N:4:DT:C5'	2.39	0.52
2:L:458:ALA:HB2	2:L:484:CYS:SG	2.49	0.52
2:J:375:ALA:O	2:J:376:LEU:O	2.27	0.52
2:I:513:ILE:CD1	2:I:514:LYS:H	2.22	0.52
2:K:447:ILE:HG13	2:K:476:LEU:CB	2.39	0.52
2:C:539:VAL:HG12	2:C:540:GLN:N	2.24	0.52
2:D:530:ASP:OD1	2:G:533:LEU:HD21	2.09	0.52
2:D:395:TRP:CZ2	2:D:570:ARG:NH1	2.75	0.52
2:E:432:ILE:HD12	2:E:541:THR:HG21	1.91	0.52
2:B:478:ASP:HB3	2:C:494:ASN:ND2	2.24	0.52
2:K:457:PHE:O	2:K:457:PHE:CD2	2.62	0.52
2:L:446:LEU:HD13	2:L:559:ILE:CB	2.38	0.52
2:C:500:PRO:HA	2:C:514:LYS:HA	1.92	0.52
2:D:401:PHE:HE2	2:D:544:PHE:HE2	1.58	0.52
2:E:525:ASP:OD2	2:E:543:ARG:NH1	2.42	0.52
2:B:311:PHE:CE1	2:B:348:PHE:HB2	2.45	0.52
2:D:452:GLY:HA3	2:D:474:ALA:O	2.09	0.52
1:M:3:DT:C2'	1:M:4:DT:H5"	2.39	0.52
2:A:442:LEU:HD12	2:A:559:ILE:HG13	1.90	0.52
2:G:424:PRO:HA	2:G:497:ASP:O	2.09	0.52
2:F:453:SER:N	2:F:472:THR:HG21	2.25	0.52
2:A:376:LEU:HD12	2:A:380:ALA:HB1	1.92	0.52
2:L:445:SER:O	2:L:446:LEU:CD2	2.57	0.52
2:L:428:CYS:SG	2:L:539:VAL:HG22	2.50	0.52
2:D:530:ASP:CG	2:G:533:LEU:CD2	2.78	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:460:HIS:CG	2:L:460:HIS:O	2.63	0.52
2:L:494:ASN:HB3	2:L:499:TYR:HA	1.92	0.52
2:B:513:ILE:HD12	2:B:514:LYS:H	1.75	0.52
2:L:483:ALA:C	2:L:485:TRP:N	2.63	0.52
2:E:506:LYS:O	2:E:507:HIS:HB2	2.09	0.52
2:D:439:LYS:HB2	5:D:4:ADP:O2B	2.09	0.52
2:C:412:PHE:HA	2:C:542:PHE:CZ	2.45	0.52
2:I:490:THR:HG22	2:I:491:TYR:CD2	2.45	0.52
2:H:401:PHE:HE2	2:H:544:PHE:HE2	1.57	0.52
2:K:370:ARG:HH11	2:K:370:ARG:HG2	1.75	0.52
2:L:401:PHE:CE2	2:L:443:CYS:SG	3.03	0.52
2:L:417:LYS:HE3	2:L:576:ASP:OD1	2.10	0.52
2:K:432:ILE:HA	2:K:522:SER:O	2.10	0.52
2:K:306:LEU:CD2	2:K:306:LEU:H	2.19	0.52
2:B:316:MET:HE2	2:B:361:CYS:HB2	1.89	0.52
2:G:367:HIS:CE1	2:L:328:GLU:HB3	2.45	0.52
2:J:440:SER:O	2:J:444:ASN:HB2	2.10	0.52
2:K:543:ARG:HH11	2:K:543:ARG:HG2	1.74	0.52
2:A:432:ILE:HA	2:A:522:SER:O	2.09	0.52
2:G:533:LEU:HD12	2:G:536:HIS:ND1	2.25	0.52
2:A:377:SER:O	2:A:378:MET:C	2.48	0.52
2:I:444:ASN:ND2	2:J:500:PRO:HD2	2.25	0.52
1:N:5:DT:P	2:J:506:LYS:HE2	2.50	0.51
2:L:399:LEU:HD13	2:L:409:LEU:CD2	2.41	0.51
2:K:457:PHE:O	2:K:457:PHE:CG	2.63	0.51
2:L:434:PRO:HD2	2:L:437:THR:CG2	2.39	0.51
2:C:497:ASP:HB3	2:C:499:TYR:CD2	2.45	0.51
2:D:446:LEU:HD23	2:D:519:LEU:HD11	1.92	0.51
2:A:485:TRP:CE3	2:A:526:VAL:HG11	2.45	0.51
2:I:319:TRP:HH2	2:I:334:GLU:HB3	1.75	0.51
1:N:3:DT:C1'	1:N:4:DT:H5"	2.40	0.51
2:B:455:LEU:HD21	2:B:469:LEU:CD2	2.40	0.51
2:A:410:ILE:HG23	2:A:411:THR:N	2.26	0.51
5:B:2:ADP:H5'1	2:C:425:LYS:CD	2.40	0.51
2:F:376:LEU:HD23	2:F:376:LEU:H	1.68	0.51
2:E:453:SER:O	2:E:475:ALA:HA	2.10	0.51
2:B:490:THR:HG22	2:B:491:TYR:CE2	2.45	0.51
2:B:476:LEU:HD22	2:B:477:VAL:N	2.26	0.51
2:B:485:TRP:CE3	2:B:526:VAL:HG11	2.46	0.51
2:B:370:ARG:NH1	2:B:370:ARG:HG2	2.22	0.51
2:D:454:VAL:HG22	2:D:476:LEU:HD12	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:316:MET:HE2	2:D:361:CYS:HB2	1.92	0.51
2:H:571:LEU:CD2	2:H:574:ARG:HE	2.23	0.51
2:H:419:TRP:CE2	2:H:517:PRO:HB3	2.45	0.51
2:C:378:MET:HB3	2:C:379:PRO:HD3	1.92	0.51
2:A:493:ARG:O	2:A:496:LEU:HB2	2.10	0.51
2:L:395:TRP:HB2	2:L:567:PHE:HA	1.93	0.51
2:I:441:MET:C	2:I:441:MET:SD	2.89	0.51
2:J:525:ASP:OD1	2:J:527:GLN:HB2	2.11	0.51
2:H:378:MET:CE	2:H:473:ARG:NH1	2.74	0.51
2:F:384:ALA:O	2:F:388:LEU:HD23	2.10	0.51
2:E:313:PHE:CE2	2:E:317:VAL:HG21	2.45	0.51
2:L:492:LEU:CD1	2:L:501:VAL:HG11	2.39	0.51
2:H:344:ASN:O	2:H:347:ALA:N	2.44	0.51
2:E:490:THR:HG22	2:E:491:TYR:CD2	2.46	0.51
2:J:497:ASP:OD1	2:J:538:ARG:NH1	2.44	0.51
2:E:354:GLN:O	2:E:358:VAL:HG23	2.11	0.51
2:A:456:SER:C	2:A:465:TRP:CE3	2.84	0.51
1:M:2:DT:C5	1:M:3:DT:C4	2.99	0.51
2:K:432:ILE:HD12	2:K:541:THR:CG2	2.41	0.51
2:L:434:PRO:CD	2:L:437:THR:HG21	2.38	0.51
2:L:499:TYR:HB2	2:L:500:PRO:CD	2.40	0.51
2:K:306:LEU:N	2:K:306:LEU:HD22	2.21	0.51
2:K:353:SER:O	2:K:357:HIS:CD2	2.64	0.51
2:D:362:ALA:O	2:D:366:ARG:HG2	2.11	0.51
2:C:502:SER:O	2:C:503:ILE:HD13	2.11	0.51
2:J:374:GLN:OE1	2:J:374:GLN:HA	2.10	0.51
2:D:497:ASP:CG	2:D:538:ARG:HE	2.15	0.51
2:L:432:ILE:HG22	2:L:433:GLY:N	2.26	0.51
2:F:431:PHE:CD2	2:F:443:CYS:SG	3.04	0.51
2:J:513:ILE:HG23	2:J:514:LYS:N	2.25	0.51
2:J:435:PRO:O	2:J:436:ASN:HB2	2.10	0.51
2:A:461:LYS:C	2:A:463:HIS:N	2.64	0.50
1:N:3:DT:C2'	1:N:4:DT:H5"	2.41	0.50
2:H:344:ASN:O	2:H:347:ALA:HB3	2.11	0.50
2:D:384:ALA:O	2:D:388:LEU:HD23	2.11	0.50
2:D:414:ASN:O	2:D:418:LEU:HD13	2.11	0.50
2:K:505:ARG:NE	2:K:511:VAL:HG23	2.26	0.50
2:B:384:ALA:O	2:B:388:LEU:HD23	2.10	0.50
2:L:437:THR:HG23	2:L:546:GLN:N	2.26	0.50
2:G:439:LYS:HB2	5:G:7:ADP:O2B	2.12	0.50
2:C:438:GLY:O	2:C:441:MET:HB3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:363:THR:HG22	2:L:367:HIS:CD2	2.46	0.50
1:N:4:DT:H1'	1:N:5:DT:O4'	2.10	0.50
2:E:366:ARG:O	2:E:367:HIS:C	2.49	0.50
2:I:381:TYR:O	2:I:384:ALA:N	2.45	0.50
2:G:364:MET:O	2:G:367:HIS:HB2	2.12	0.50
2:H:401:PHE:HE2	2:H:544:PHE:CE2	2.29	0.50
2:H:331:ILE:HD12	2:H:362:ALA:HB2	1.92	0.50
2:I:460:HIS:HA	2:I:465:TRP:CG	2.46	0.50
2:A:461:LYS:O	2:A:463:HIS:N	2.44	0.50
2:G:349:LEU:HA	2:G:354:GLN:HE21	1.76	0.50
2:D:476:LEU:HD22	2:D:476:LEU:C	2.31	0.50
2:F:493:ARG:HD3	2:F:534:TYR:CE2	2.46	0.50
2:E:316:MET:O	2:E:319:TRP:HB3	2.12	0.50
2:A:477:VAL:HG21	2:A:488:PHE:HZ	1.77	0.50
2:F:313:PHE:O	2:F:314:GLY:C	2.50	0.50
2:I:434:PRO:O	2:I:437:THR:HG23	2.12	0.50
2:L:529:GLU:HG3	2:L:531:ARG:HG3	1.94	0.50
2:A:457:PHE:O	2:A:460:HIS:ND1	2.44	0.50
2:J:417:LYS:HG3	2:J:575:LEU:O	2.10	0.50
2:F:316:MET:CE	2:F:361:CYS:HB2	2.41	0.50
2:L:351:THR:HG21	2:L:357:HIS:CD2	2.47	0.50
2:J:377:SER:O	2:J:378:MET:C	2.51	0.50
1:N:4:DT:H2"	1:N:5:DT:O5'	2.11	0.50
2:B:409:LEU:HG	2:B:413:ILE:CD1	2.41	0.50
2:K:432:ILE:HD12	2:K:541:THR:HG21	1.94	0.50
2:H:511:VAL:HG12	2:H:513:ILE:HG22	1.93	0.50
2:F:438:GLY:CA	5:F:6:ADP:H4'	2.40	0.50
2:I:494:ASN:O	2:I:497:ASP:HB2	2.12	0.50
2:I:427:ASN:HD21	2:I:517:PRO:HA	1.76	0.50
2:G:513:ILE:CD1	2:G:514:LYS:H	2.24	0.50
2:H:308:THR:O	2:H:310:LYS:N	2.45	0.50
2:C:502:SER:C	2:C:503:ILE:HD13	2.32	0.50
2:F:337:LEU:C	2:F:339:ALA:H	2.14	0.50
2:L:434:PRO:HG2	2:L:437:THR:CG2	2.42	0.50
2:K:441:MET:CE	2:K:559:ILE:H	2.16	0.50
2:D:399:LEU:O	2:D:402:PHE:N	2.45	0.50
2:F:335:TYR:CE2	2:F:345:ALA:HA	2.46	0.50
2:K:552:SER:C	2:K:554:GLU:H	2.14	0.50
2:J:418:LEU:HD12	2:J:418:LEU:H	1.75	0.50
2:K:446:LEU:HB2	2:K:564:TRP:CZ2	2.47	0.50
2:E:363:THR:O	2:E:367:HIS:CD2	2.65	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:513:ILE:CG1	2:K:514:LYS:N	2.75	0.49
2:B:492:LEU:HD13	2:B:492:LEU:N	2.27	0.49
2:D:378:MET:O	2:D:382:ILE:HG13	2.12	0.49
2:J:414:ASN:O	2:J:418:LEU:HD13	2.11	0.49
2:G:485:TRP:CD2	2:G:526:VAL:HG11	2.47	0.49
2:L:418:LEU:HD22	2:L:426:LYS:HD3	1.93	0.49
2:K:541:THR:C	2:K:542:PHE:HD2	2.15	0.49
2:F:362:ALA:O	2:F:363:THR:C	2.50	0.49
2:L:416:LEU:HD12	2:L:419:TRP:CE3	2.47	0.49
2:G:523:ASN:N	2:G:523:ASN:ND2	2.60	0.49
2:G:502:SER:O	2:G:503:ILE:HD13	2.12	0.49
2:L:434:PRO:HD3	2:L:545:GLU:OE2	2.11	0.49
2:I:441:MET:SD	2:I:442:LEU:N	2.85	0.49
2:C:376:LEU:HD23	2:C:381:TYR:CA	2.37	0.49
2:J:509:ALA:O	2:J:510:ALA:O	2.31	0.49
2:D:489:ASP:CA	2:D:535:LEU:HD21	2.40	0.49
2:K:526:VAL:HG12	2:K:532:TYR:CD1	2.46	0.49
2:E:337:LEU:C	2:E:339:ALA:H	2.15	0.49
2:B:479:ASP:OD2	2:C:538:ARG:NH2	2.45	0.49
2:G:499:TYR:HB3	2:G:500:PRO:HD2	1.94	0.49
2:B:492:LEU:CD1	2:B:492:LEU:N	2.75	0.49
2:A:525:ASP:OD2	2:A:543:ARG:NH1	2.45	0.49
2:B:494:ASN:ND2	2:B:494:ASN:H	2.03	0.49
2:B:334:GLU:O	2:B:337:LEU:HB2	2.12	0.49
1:N:3:DT:H2"	1:N:4:DT:H5"	1.94	0.49
2:E:462:SER:O	2:E:464:PHE:N	2.46	0.49
2:C:427:ASN:ND2	2:C:517:PRO:HA	2.27	0.49
2:B:398:ILE:HD12	2:B:567:PHE:HB2	1.94	0.49
2:B:497:ASP:HB3	2:B:499:TYR:CD2	2.47	0.49
2:A:523:ASN:OD1	2:A:524:ILE:N	2.45	0.49
2:K:354:GLN:OE1	2:L:364:MET:HG2	2.13	0.49
2:H:488:PHE:HB3	2:H:496:LEU:HD11	1.94	0.49
2:D:398:ILE:HD11	2:D:564:TRP:CD2	2.47	0.49
2:J:459:ASN:C	2:J:461:LYS:H	2.16	0.49
2:L:447:ILE:CG1	2:L:564:TRP:CE2	2.87	0.49
2:B:529:GLU:CG	2:B:531:ARG:HE	2.25	0.49
2:G:378:MET:HB3	2:G:379:PRO:HD3	1.95	0.49
2:H:308:THR:C	2:H:310:LYS:H	2.16	0.49
2:H:348:PHE:CD2	2:H:349:LEU:HD23	2.48	0.49
2:D:548:CYS:O	2:D:550:ASP:N	2.45	0.49
2:A:466:LEU:O	2:A:469:LEU:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:424:PRO:HB3	2:D:499:TYR:CE2	2.48	0.49
2:H:378:MET:O	2:H:382:ILE:HG13	2.13	0.49
2:K:357:HIS:O	2:K:361:CYS:N	2.39	0.49
2:F:513:ILE:CG1	2:F:514:LYS:H	2.26	0.49
2:A:485:TRP:CD2	2:A:526:VAL:HG11	2.47	0.49
2:F:533:LEU:HA	2:F:536:HIS:CE1	2.48	0.49
2:A:432:ILE:HD13	2:A:524:ILE:O	2.12	0.49
2:G:377:SER:O	2:G:380:ALA:N	2.45	0.49
2:L:545:GLU:N	2:L:546:GLN:OE1	2.46	0.49
2:L:496:LEU:HD13	2:L:538:ARG:CD	2.41	0.49
2:L:382:ILE:CG2	2:L:568:PHE:CD1	2.96	0.49
1:M:3:DT:H2"	1:M:4:DT:H5"	1.95	0.49
2:L:483:ALA:O	2:L:485:TRP:N	2.46	0.49
2:I:427:ASN:HD21	2:I:517:PRO:CA	2.26	0.49
2:J:441:MET:HE1	2:J:559:ILE:HB	1.95	0.49
2:E:462:SER:C	2:E:464:PHE:H	2.17	0.49
2:H:446:LEU:HB2	2:H:564:TRP:CZ2	2.48	0.49
2:L:567:PHE:HD2	2:L:568:PHE:HD2	1.60	0.48
2:K:464:PHE:C	2:K:466:LEU:N	2.66	0.48
2:C:453:SER:CB	2:C:472:THR:HG21	2.37	0.48
2:F:438:GLY:HA2	5:F:6:ADP:C4'	2.42	0.48
2:B:316:MET:O	2:B:319:TRP:HB3	2.13	0.48
2:C:559:ILE:HG23	2:C:563:ASP:HB2	1.94	0.48
2:F:494:ASN:C	2:F:496:LEU:N	2.65	0.48
2:J:533:LEU:HA	2:J:536:HIS:CE1	2.49	0.48
2:K:362:ALA:O	2:K:363:THR:C	2.51	0.48
2:G:435:PRO:O	2:G:436:ASN:HB2	2.13	0.48
2:A:446:LEU:HD13	2:A:564:TRP:CZ2	2.49	0.48
2:A:403:ASN:O	2:A:404:TYR:C	2.51	0.48
2:E:395:TRP:CE2	2:E:570:ARG:NE	2.80	0.48
2:C:513:ILE:HG13	2:C:514:LYS:N	2.27	0.48
2:A:412:PHE:HA	2:A:542:PHE:CZ	2.48	0.48
2:A:328:GLU:O	2:A:329:SER:C	2.51	0.48
2:F:412:PHE:HA	2:F:542:PHE:CE1	2.48	0.48
2:F:401:PHE:HE2	2:F:544:PHE:CE2	2.32	0.48
2:J:358:VAL:HG21	2:K:364:MET:HE3	1.95	0.48
2:B:378:MET:N	2:B:379:PRO:CD	2.76	0.48
2:A:460:HIS:HA	2:A:465:TRP:CB	2.39	0.48
2:L:454:VAL:O	2:L:455:LEU:CG	2.55	0.48
2:D:513:ILE:CD1	2:D:514:LYS:H	2.17	0.48
2:A:477:VAL:HG21	2:A:488:PHE:CZ	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:427:ASN:ND2	2:I:517:PRO:CA	2.74	0.48
2:D:548:CYS:O	2:D:549:THR:C	2.51	0.48
2:H:399:LEU:HD13	2:H:409:LEU:HD22	1.96	0.48
2:J:311:PHE:CZ	2:J:313:PHE:HA	2.49	0.48
2:A:460:HIS:ND1	2:A:460:HIS:N	2.62	0.48
2:F:418:LEU:HD22	2:F:426:LYS:HG2	1.96	0.48
2:G:476:LEU:HD13	2:G:476:LEU:O	2.13	0.48
2:K:485:TRP:CD2	2:K:526:VAL:HG11	2.47	0.48
2:C:382:ILE:HD11	2:C:420:LEU:HD22	1.96	0.48
2:F:457:PHE:CZ	2:F:484:CYS:HA	2.49	0.48
2:A:347:ALA:O	2:A:350:ALA:HB3	2.13	0.48
2:C:328:GLU:O	2:C:329:SER:C	2.51	0.48
2:L:410:ILE:HG12	2:L:410:ILE:O	2.12	0.48
2:K:462:SER:C	2:K:464:PHE:N	2.67	0.48
2:I:441:MET:HE3	2:I:559:ILE:H	1.78	0.48
2:G:489:ASP:O	2:G:493:ARG:NE	2.46	0.48
2:G:453:SER:HB3	2:G:472:THR:CG2	2.43	0.48
2:I:499:TYR:HB3	2:I:500:PRO:HD2	1.94	0.48
2:B:476:LEU:HA	2:B:519:LEU:O	2.14	0.48
2:C:496:LEU:HD23	2:C:518:LEU:HD12	1.94	0.48
2:D:421:LYS:HB2	2:D:423:ILE:HD12	1.95	0.48
2:A:398:ILE:HG12	2:A:559:ILE:HD12	1.96	0.48
2:F:435:PRO:HA	5:F:6:ADP:O3B	2.14	0.48
2:L:378:MET:N	2:L:379:PRO:HD2	2.29	0.48
2:L:379:PRO:CB	2:L:577:LEU:HD22	2.41	0.48
2:I:351:THR:HG21	2:I:357:HIS:CD2	2.48	0.48
2:L:337:LEU:C	2:L:339:ALA:H	2.16	0.48
2:A:494:ASN:C	2:A:496:LEU:N	2.67	0.48
2:H:376:LEU:HB3	2:H:377:SER:H	1.42	0.48
2:D:477:VAL:HG21	2:D:488:PHE:HZ	1.79	0.48
2:G:513:ILE:CG1	2:G:514:LYS:N	2.77	0.48
2:H:401:PHE:CE2	2:H:544:PHE:CE2	3.02	0.48
2:G:386:CYS:O	2:G:387:LYS:C	2.53	0.48
2:A:384:ALA:O	2:A:388:LEU:HD23	2.14	0.48
2:C:565:LYS:O	2:C:569:VAL:HG23	2.14	0.48
2:L:434:PRO:CB	2:L:437:THR:OG1	2.62	0.48
2:L:383:LYS:HA	2:L:386:CYS:HB2	1.94	0.48
2:B:345:ALA:O	2:B:348:PHE:HB3	2.14	0.48
2:I:453:SER:CB	2:I:472:THR:HG21	2.42	0.48
2:L:398:ILE:CG2	2:L:399:LEU:N	2.76	0.48
2:L:571:LEU:O	2:L:575:LEU:HB2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:499:TYR:CB	2:L:500:PRO:CD	2.91	0.47
2:D:437:THR:OG1	2:D:439:LYS:HE2	2.14	0.47
2:H:351:THR:HG21	2:H:357:HIS:CD2	2.49	0.47
2:H:476:LEU:HD22	2:H:476:LEU:C	2.34	0.47
2:H:410:ILE:CG2	2:H:411:THR:N	2.77	0.47
2:J:526:VAL:HG12	2:J:532:TYR:CD1	2.49	0.47
2:E:373:THR:HG23	2:E:381:TYR:CE1	2.49	0.47
2:K:395:TRP:CE2	2:K:570:ARG:NE	2.83	0.47
2:D:405:GLN:O	2:D:406:ASN:HB2	2.13	0.47
2:I:552:SER:O	2:I:554:GLU:N	2.39	0.47
2:K:418:LEU:HD12	2:K:418:LEU:N	2.29	0.47
2:B:351:THR:HG21	2:B:357:HIS:CD2	2.49	0.47
2:J:328:GLU:O	2:J:329:SER:C	2.53	0.47
2:K:410:ILE:HG12	2:K:414:ASN:ND2	2.29	0.47
2:G:488:PHE:CE1	2:G:492:LEU:HD23	2.49	0.47
2:A:425:LYS:HE3	2:A:426:LYS:HE2	1.96	0.47
2:F:419:TRP:CD1	2:F:429:LEU:HG	2.48	0.47
2:D:434:PRO:O	2:D:437:THR:HG23	2.13	0.47
2:J:368:TYR:O	2:J:372:GLU:HB2	2.14	0.47
2:E:419:TRP:CZ2	2:E:519:LEU:HG	2.49	0.47
2:G:470:ALA:HA	2:G:513:ILE:HG21	1.96	0.47
2:F:562:ALA:O	2:F:565:LYS:HB3	2.15	0.47
2:L:538:ARG:CG	2:L:539:VAL:HG23	2.42	0.47
2:F:377:SER:OG	2:F:379:PRO:HD2	2.14	0.47
2:J:432:ILE:HD12	2:J:541:THR:CG2	2.44	0.47
2:J:564:TRP:O	2:J:565:LYS:C	2.52	0.47
2:E:419:TRP:CD1	2:E:429:LEU:HG	2.48	0.47
2:I:440:SER:O	2:I:444:ASN:HB2	2.14	0.47
2:J:384:ALA:O	2:J:388:LEU:HD23	2.14	0.47
2:L:438:GLY:HA3	2:L:548:CYS:CB	2.45	0.47
2:C:432:ILE:HD12	2:C:541:THR:HG21	1.97	0.47
2:H:495:ALA:O	2:H:498:GLY:N	2.48	0.47
2:E:440:SER:N	5:E:5:ADP:O1B	2.44	0.47
2:G:432:ILE:HD12	2:G:541:THR:HG21	1.96	0.47
2:J:447:ILE:HG12	2:J:519:LEU:HD12	1.96	0.47
2:F:319:TRP:HH2	2:F:334:GLU:HB3	1.80	0.47
2:C:332:ALA:HB2	2:C:358:VAL:CG1	2.43	0.47
2:I:548:CYS:O	2:I:550:ASP:N	2.47	0.47
2:K:345:ALA:O	2:K:348:PHE:HB3	2.14	0.47
2:C:533:LEU:HA	2:C:536:HIS:CE1	2.50	0.47
2:G:395:TRP:NE1	2:G:570:ARG:HD3	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:496:LEU:HD23	2:I:518:LEU:HD12	1.97	0.47
2:J:416:LEU:HD12	2:J:416:LEU:O	2.15	0.47
2:F:330:LYS:O	2:F:331:ILE:C	2.52	0.47
2:L:465:TRP:CZ2	2:L:506:LYS:HB3	2.49	0.47
2:L:532:TYR:CB	2:L:535:LEU:HD13	2.44	0.47
2:A:503:ILE:CG1	2:A:513:ILE:HG22	2.45	0.47
2:L:418:LEU:CD2	2:L:426:LYS:HD2	2.43	0.47
2:I:419:TRP:CD1	2:I:429:LEU:HG	2.50	0.47
2:H:409:LEU:HG	2:H:413:ILE:HD11	1.97	0.47
2:J:335:TYR:CE2	2:J:345:ALA:HA	2.50	0.47
2:A:565:LYS:O	2:A:569:VAL:HG23	2.15	0.47
2:A:439:LYS:HB2	5:A:1:ADP:O2B	2.15	0.47
2:A:353:SER:O	2:A:357:HIS:CD2	2.68	0.47
2:D:399:LEU:O	2:D:401:PHE:N	2.48	0.47
2:I:506:LYS:NZ	2:J:508:LYS:O	2.47	0.47
2:J:354:GLN:O	2:J:358:VAL:HG23	2.15	0.47
2:E:424:PRO:O	2:E:425:LYS:HB2	2.15	0.47
1:N:7:DT:OP1	2:L:465:TRP:NE1	2.46	0.47
2:I:505:ARG:CZ	2:I:511:VAL:HG23	2.44	0.47
2:D:541:THR:CG2	2:D:542:PHE:N	2.78	0.47
2:F:370:ARG:HG2	2:F:370:ARG:HH11	1.80	0.47
2:A:441:MET:O	2:A:442:LEU:C	2.52	0.47
2:C:453:SER:HA	2:D:512:GLN:HE22	1.80	0.47
2:I:329:SER:HA	2:J:367:HIS:ND1	2.30	0.47
2:F:327:GLU:O	2:F:328:GLU:C	2.52	0.47
2:A:370:ARG:HH11	2:F:329:SER:CB	2.28	0.47
2:E:425:LYS:HE2	2:E:538:ARG:CZ	2.45	0.47
2:A:555:GLN:HA	2:A:556:PRO:HD2	1.73	0.47
2:D:398:ILE:HD12	2:D:567:PHE:HB2	1.97	0.47
2:F:490:THR:HG22	2:F:491:TYR:CD2	2.49	0.47
2:B:523:ASN:ND2	4:B:42:CL:CL	2.85	0.46
1:M:3:DT:H2"	1:M:4:DT:C5'	2.45	0.46
2:B:325:TYR:HE1	2:B:334:GLU:HG2	1.76	0.46
2:K:377:SER:CB	2:K:379:PRO:HD2	2.44	0.46
2:L:416:LEU:CD1	2:L:419:TRP:CE3	2.99	0.46
2:F:328:GLU:O	2:F:329:SER:C	2.53	0.46
2:C:478:ASP:HB3	2:D:494:ASN:ND2	2.30	0.46
2:K:409:LEU:HG	2:K:413:ILE:HG13	1.97	0.46
2:J:361:CYS:O	2:J:365:VAL:HG23	2.15	0.46
2:B:453:SER:O	2:B:475:ALA:HA	2.15	0.46
2:A:357:HIS:O	2:A:358:VAL:C	2.53	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:441:MET:HE3	2:D:559:ILE:H	1.81	0.46
2:F:321:TYR:CD1	2:F:321:TYR:C	2.89	0.46
2:K:317:VAL:O	2:K:318:GLN:C	2.53	0.46
2:J:501:VAL:CG2	2:J:502:SER:N	2.78	0.46
2:I:418:LEU:HG	2:I:423:ILE:HD13	1.96	0.46
2:B:399:LEU:HD13	2:B:409:LEU:HD22	1.98	0.46
2:B:434:PRO:O	2:B:437:THR:HG23	2.15	0.46
2:H:412:PHE:HA	2:H:542:PHE:CZ	2.50	0.46
2:A:447:ILE:HG12	2:A:519:LEU:HD12	1.97	0.46
2:L:380:ALA:HA	2:L:383:LYS:HG2	1.98	0.46
2:K:453:SER:OG	2:K:472:THR:HG21	2.15	0.46
2:H:425:LYS:HE3	2:H:497:ASP:OD1	2.16	0.46
2:H:425:LYS:HE2	2:H:537:SER:O	2.15	0.46
2:D:325:TYR:HE1	2:D:334:GLU:HG2	1.77	0.46
2:A:493:ARG:HD3	2:A:534:TYR:CE2	2.50	0.46
2:I:377:SER:H	2:I:380:ALA:HB3	1.80	0.46
2:L:476:LEU:HD22	2:L:477:VAL:N	2.27	0.46
2:I:331:ILE:HG22	2:I:332:ALA:N	2.30	0.46
2:K:533:LEU:HD12	2:K:536:HIS:ND1	2.30	0.46
2:L:385:ARG:CZ	2:L:450:LEU:O	2.64	0.46
2:K:476:LEU:HD22	2:K:477:VAL:N	2.30	0.46
2:C:465:TRP:HZ2	2:C:487:TYR:CE2	2.33	0.46
2:J:437:THR:OG1	2:J:439:LYS:HE2	2.16	0.46
2:A:316:MET:HE2	2:A:361:CYS:HB2	1.97	0.46
2:B:543:ARG:O	2:B:544:PHE:HD1	1.99	0.46
2:H:418:LEU:CD1	2:H:418:LEU:N	2.78	0.46
2:L:321:TYR:C	2:L:321:TYR:CD1	2.88	0.46
2:L:442:LEU:HD13	2:L:557:PHE:O	2.16	0.46
2:L:380:ALA:O	2:L:383:LYS:N	2.49	0.46
2:B:316:MET:CE	2:B:361:CYS:HB2	2.45	0.46
2:I:327:GLU:O	2:I:328:GLU:C	2.54	0.46
2:B:499:TYR:HB3	2:B:500:PRO:CD	2.44	0.46
2:H:488:PHE:HD1	2:H:496:LEU:HD21	1.80	0.46
2:H:559:ILE:HG22	2:H:560:THR:H	1.80	0.46
2:G:379:PRO:O	2:G:383:LYS:N	2.46	0.46
2:J:404:TYR:O	2:J:546:GLN:HG3	2.14	0.46
2:C:526:VAL:HG12	2:C:532:TYR:CD1	2.51	0.46
2:L:382:ILE:HG21	2:L:568:PHE:CE1	2.51	0.46
2:J:425:LYS:O	2:J:538:ARG:HA	2.16	0.46
2:I:370:ARG:O	2:I:373:THR:N	2.49	0.46
2:I:399:LEU:HD13	2:I:409:LEU:HD22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:499:TYR:CD1	2:L:500:PRO:HD2	2.52	0.45
2:A:525:ASP:C	2:A:525:ASP:OD1	2.55	0.45
2:H:500:PRO:HA	2:H:514:LYS:HA	1.98	0.45
2:B:361:CYS:O	2:B:365:VAL:HG23	2.15	0.45
2:I:419:TRP:CE2	2:I:517:PRO:HB3	2.51	0.45
2:G:497:ASP:OD1	2:G:538:ARG:HG2	2.16	0.45
2:F:348:PHE:CD2	2:F:349:LEU:HD23	2.51	0.45
2:E:505:ARG:NH1	2:E:511:VAL:HG23	2.31	0.45
2:J:572:TRP:CE2	2:J:577:LEU:HB3	2.51	0.45
2:I:315:THR:HB	2:I:344:ASN:ND2	2.31	0.45
2:H:377:SER:CB	2:H:379:PRO:HD2	2.46	0.45
2:H:378:MET:HB3	2:H:379:PRO:HD3	1.98	0.45
2:G:571:LEU:CD2	2:G:574:ARG:HE	2.29	0.45
2:B:467:ALA:O	2:B:468:SER:C	2.53	0.45
2:A:455:LEU:HB3	2:A:465:TRP:CE3	2.51	0.45
2:H:499:TYR:HB3	2:H:500:PRO:HD2	1.98	0.45
2:J:453:SER:CB	2:J:472:THR:HG21	2.38	0.45
2:A:367:HIS:ND1	2:F:329:SER:HA	2.31	0.45
2:I:351:THR:HG21	2:I:357:HIS:NE2	2.31	0.45
2:D:440:SER:O	2:D:444:ASN:HB2	2.16	0.45
2:L:560:THR:HG1	2:L:563:ASP:CG	2.20	0.45
2:A:351:THR:HG21	2:A:357:HIS:CD2	2.51	0.45
2:L:362:ALA:O	2:L:363:THR:C	2.54	0.45
2:H:443:CYS:SG	2:H:519:LEU:HD13	2.56	0.45
2:K:332:ALA:HB2	2:K:358:VAL:HG11	1.99	0.45
2:L:559:ILE:CG2	2:L:560:THR:N	2.79	0.45
2:L:417:LYS:HB3	2:L:418:LEU:HD12	1.97	0.45
5:C:3:ADP:H5'1	2:D:425:LYS:HD2	1.99	0.45
2:K:361:CYS:O	2:K:365:VAL:HG23	2.16	0.45
2:D:453:SER:CB	2:D:472:THR:HG21	2.46	0.45
2:A:372:GLU:O	2:A:376:LEU:CD2	2.65	0.45
2:E:332:ALA:HB2	2:E:358:VAL:HG11	1.99	0.45
2:B:501:VAL:HG11	2:B:515:ALA:HB2	1.98	0.45
2:G:459:ASN:O	2:G:465:TRP:HB3	2.17	0.45
2:L:387:LYS:HD2	2:L:387:LYS:O	2.16	0.45
2:L:572:TRP:CD1	2:L:572:TRP:C	2.90	0.45
2:A:469:LEU:HD12	2:A:503:ILE:HD11	1.99	0.45
2:A:531:ARG:HH12	2:K:528:ALA:N	2.14	0.45
1:N:5:DT:OP1	2:J:506:LYS:NZ	2.43	0.45
2:J:447:ILE:HG13	2:J:476:LEU:CB	2.47	0.45
2:C:559:ILE:CG2	2:C:560:THR:N	2.77	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:378:MET:N	2:D:379:PRO:CD	2.79	0.45
2:K:523:ASN:N	2:K:523:ASN:ND2	2.65	0.45
2:F:562:ALA:O	2:F:565:LYS:N	2.50	0.45
2:L:387:LYS:CD	2:L:387:LYS:O	2.64	0.45
2:J:551:GLU:O	2:J:552:SER:C	2.55	0.45
2:L:434:PRO:HG3	2:L:545:GLU:OE1	2.16	0.45
2:A:463:HIS:HB3	2:A:466:LEU:HD12	1.99	0.45
2:L:454:VAL:CG1	2:L:455:LEU:N	2.51	0.45
2:F:432:ILE:HA	2:F:522:SER:O	2.16	0.45
2:C:373:THR:C	2:C:375:ALA:N	2.70	0.45
2:K:457:PHE:CZ	2:K:484:CYS:HA	2.52	0.45
2:A:372:GLU:O	2:A:376:LEU:HD22	2.16	0.45
2:E:489:ASP:O	2:E:493:ARG:NE	2.47	0.45
2:L:420:LEU:C	2:L:422:GLY:H	2.20	0.45
2:L:521:THR:O	2:L:522:SER:HB2	2.17	0.45
2:L:466:LEU:CG	2:L:467:ALA:N	2.73	0.45
2:D:533:LEU:O	2:D:536:HIS:ND1	2.50	0.45
2:B:319:TRP:HH2	2:B:334:GLU:HB3	1.81	0.45
2:F:418:LEU:H	2:F:418:LEU:CD1	2.29	0.45
2:A:556:PRO:HB2	2:A:557:PHE:H	1.51	0.45
2:D:419:TRP:CZ2	2:D:519:LEU:HG	2.51	0.45
2:E:484:CYS:SG	2:E:488:PHE:HE2	2.40	0.45
2:L:559:ILE:HG22	2:L:560:THR:N	2.31	0.45
2:G:319:TRP:HH2	2:G:334:GLU:HB3	1.82	0.45
2:I:513:ILE:HD12	2:I:514:LYS:H	1.82	0.45
2:I:485:TRP:CD2	2:I:526:VAL:HG11	2.51	0.45
2:I:553:GLY:O	2:I:554:GLU:C	2.54	0.45
2:H:519:LEU:HD23	2:H:519:LEU:HA	1.84	0.45
2:E:550:ASP:O	2:E:551:GLU:C	2.55	0.45
2:A:546:GLN:HA	2:A:547:PRO:HD3	1.75	0.45
2:L:405:GLN:OE1	2:L:546:GLN:OE1	2.35	0.45
2:L:383:LYS:O	2:L:386:CYS:N	2.50	0.45
2:A:441:MET:O	2:A:445:SER:N	2.23	0.45
2:F:441:MET:CB	5:F:6:ADP:H1'	2.47	0.45
2:D:328:GLU:O	2:D:329:SER:C	2.55	0.45
2:K:493:ARG:HD3	2:K:534:TYR:CE2	2.52	0.45
2:K:534:TYR:CZ	2:K:538:ARG:CZ	3.00	0.45
2:D:462:SER:O	2:D:464:PHE:N	2.50	0.45
2:L:505:ARG:H	2:L:505:ARG:HG2	1.58	0.44
2:A:523:ASN:OD1	2:A:524:ILE:HG13	2.17	0.44
5:H:8:ADP:O2A	2:I:425:LYS:HD2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:328:GLU:O	2:K:329:SER:C	2.55	0.44
2:D:395:TRP:CD2	2:D:570:ARG:HD2	2.52	0.44
2:L:493:ARG:NH2	2:L:534:TYR:HD1	2.13	0.44
2:J:564:TRP:O	2:J:567:PHE:HB3	2.17	0.44
2:E:497:ASP:OD1	2:E:538:ARG:NH1	2.51	0.44
2:F:505:ARG:NH2	2:F:509:ALA:O	2.43	0.44
2:K:404:TYR:C	2:K:404:TYR:CD2	2.90	0.44
2:E:360:ASP:O	2:E:361:CYS:C	2.55	0.44
2:C:475:ALA:HB3	2:C:518:LEU:CD2	2.48	0.44
2:G:466:LEU:HD22	2:G:469:LEU:CD1	2.47	0.44
2:K:434:PRO:O	2:K:437:THR:HG23	2.17	0.44
2:B:552:SER:O	2:B:553:GLY:C	2.55	0.44
2:A:494:ASN:C	2:A:496:LEU:H	2.19	0.44
2:B:494:ASN:ND2	2:B:494:ASN:N	2.61	0.44
2:I:376:LEU:HD12	2:I:380:ALA:CB	2.39	0.44
2:I:465:TRP:O	2:I:466:LEU:HD23	2.18	0.44
2:I:551:GLU:O	2:I:552:SER:CB	2.65	0.44
2:L:427:ASN:ND2	2:L:517:PRO:HA	2.32	0.44
2:B:495:ALA:O	2:B:498:GLY:N	2.46	0.44
2:E:432:ILE:HD12	2:E:541:THR:CG2	2.47	0.44
2:K:485:TRP:CD2	2:K:526:VAL:CG1	3.00	0.44
2:G:377:SER:O	2:G:378:MET:C	2.55	0.44
2:C:378:MET:O	2:C:382:ILE:HG13	2.16	0.44
2:J:449:PHE:CE2	2:J:568:PHE:CD2	3.06	0.44
2:A:534:TYR:CZ	2:A:538:ARG:NH1	2.72	0.44
2:L:476:LEU:C	2:L:476:LEU:HD13	2.38	0.44
2:A:382:ILE:HD11	2:A:420:LEU:CD2	2.46	0.44
2:A:458:ALA:HB2	2:B:491:TYR:HB3	1.99	0.44
2:A:378:MET:N	2:A:473:ARG:HH21	2.14	0.44
2:E:395:TRP:CZ2	2:E:570:ARG:NE	2.86	0.44
2:I:505:ARG:CZ	2:I:511:VAL:CG2	2.95	0.44
2:B:533:LEU:HA	2:B:536:HIS:CE1	2.53	0.44
2:B:383:LYS:O	2:B:386:CYS:HB2	2.17	0.44
2:H:351:THR:HG21	2:H:357:HIS:NE2	2.32	0.44
2:K:379:PRO:O	2:K:382:ILE:N	2.50	0.44
2:J:464:PHE:HE1	2:J:505:ARG:O	2.01	0.44
2:D:418:LEU:HD12	2:D:418:LEU:N	2.33	0.44
2:I:465:TRP:CD2	2:I:465:TRP:O	2.70	0.44
2:G:465:TRP:NE1	2:G:466:LEU:HG	2.32	0.44
2:I:459:ASN:C	2:I:461:LYS:H	2.21	0.44
2:L:437:THR:CG2	2:L:546:GLN:N	2.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:499:TYR:HD1	2:L:500:PRO:HD3	1.83	0.44
2:L:535:LEU:HG	2:L:538:ARG:NH2	2.33	0.44
2:L:382:ILE:HG21	2:L:568:PHE:CD1	2.53	0.44
2:E:432:ILE:HA	2:E:522:SER:O	2.18	0.44
2:I:497:ASP:CG	2:I:538:ARG:HE	2.21	0.44
2:E:485:TRP:CD2	2:E:526:VAL:CG1	3.00	0.44
2:B:315:THR:HB	2:B:344:ASN:ND2	2.32	0.44
2:C:413:ILE:HD13	2:C:571:LEU:HD22	1.99	0.44
2:J:351:THR:HG21	2:J:357:HIS:CD2	2.52	0.44
2:K:462:SER:O	2:K:464:PHE:N	2.50	0.44
2:K:483:ALA:O	2:K:486:ARG:HB3	2.18	0.44
2:L:458:ALA:O	2:L:459:ASN:C	2.56	0.44
2:A:427:ASN:ND2	2:A:517:PRO:HA	2.32	0.44
2:F:493:ARG:O	2:F:496:LEU:HB2	2.18	0.44
2:A:417:LYS:HG3	2:A:575:LEU:O	2.17	0.44
2:J:370:ARG:HG2	2:J:370:ARG:HH11	1.83	0.44
2:G:428:CYS:C	2:G:429:LEU:HD23	2.38	0.44
2:D:482:HIS:CE1	2:D:524:ILE:HD13	2.53	0.44
2:L:405:GLN:NE2	2:L:544:PHE:HB3	2.33	0.44
2:J:432:ILE:O	2:J:543:ARG:HA	2.17	0.44
2:F:525:ASP:OD2	2:F:543:ARG:NH1	2.51	0.44
2:F:541:THR:C	2:F:542:PHE:HD2	2.21	0.44
2:L:364:MET:O	2:L:367:HIS:HB2	2.18	0.44
2:A:367:HIS:HE1	2:F:328:GLU:CB	2.30	0.44
2:E:552:SER:O	2:E:553:GLY:C	2.55	0.44
2:A:567:PHE:O	2:A:571:LEU:HB2	2.18	0.44
2:A:497:ASP:OD2	2:A:538:ARG:NH2	2.50	0.44
2:A:503:ILE:HG13	2:A:513:ILE:HG22	2.00	0.44
2:H:513:ILE:HD12	2:H:514:LYS:N	2.33	0.44
2:A:476:LEU:HD23	2:A:519:LEU:HB3	1.99	0.44
2:D:395:TRP:NE1	2:D:396:LYS:HG3	2.33	0.44
2:J:427:ASN:HD21	2:J:517:PRO:HA	1.82	0.44
2:I:464:PHE:CD2	2:I:506:LYS:CG	2.99	0.44
2:B:441:MET:CE	2:B:559:ILE:H	2.31	0.44
2:J:344:ASN:O	2:J:347:ALA:HB3	2.17	0.44
2:L:315:THR:HB	2:L:344:ASN:ND2	2.32	0.44
2:L:488:PHE:C	2:L:538:ARG:HH22	2.22	0.43
1:M:4:DT:H2"	1:M:5:DT:O5'	2.18	0.43
2:K:316:MET:O	2:K:319:TRP:HB3	2.18	0.43
2:D:532:TYR:HB3	2:D:535:LEU:HD12	2.00	0.43
2:K:404:TYR:OH	2:K:547:PRO:O	2.26	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:418:LEU:HG	2:H:423:ILE:HD12	1.99	0.43
2:E:493:ARG:HD3	2:E:534:TYR:CE2	2.52	0.43
2:E:457:PHE:CZ	2:E:484:CYS:HA	2.53	0.43
2:L:436:ASN:C	2:L:438:GLY:N	2.71	0.43
2:D:401:PHE:O	2:D:404:TYR:HB3	2.18	0.43
2:L:534:TYR:C	2:L:536:HIS:H	2.21	0.43
2:H:490:THR:HG22	2:H:491:TYR:CD2	2.53	0.43
2:E:337:LEU:C	2:E:339:ALA:N	2.71	0.43
2:E:369:LEU:HA	2:E:369:LEU:HD23	1.75	0.43
2:L:348:PHE:CZ	2:L:354:GLN:HB3	2.53	0.43
2:F:377:SER:O	2:F:378:MET:C	2.55	0.43
2:K:453:SER:H	2:K:472:THR:HG21	1.83	0.43
2:A:459:ASN:O	2:A:465:TRP:HB3	2.18	0.43
2:E:325:TYR:HE1	2:E:334:GLU:HG2	1.79	0.43
2:K:316:MET:HE2	2:K:361:CYS:HB2	2.00	0.43
2:B:447:ILE:HG13	2:B:476:LEU:CB	2.48	0.43
2:L:345:ALA:O	2:L:348:PHE:HB3	2.17	0.43
2:C:337:LEU:C	2:C:339:ALA:H	2.22	0.43
2:K:399:LEU:O	2:K:400:THR:C	2.55	0.43
2:J:330:LYS:O	2:J:331:ILE:C	2.56	0.43
2:D:551:GLU:O	2:D:552:SER:CB	2.66	0.43
2:L:567:PHE:HD2	2:L:568:PHE:CD2	2.36	0.43
2:F:378:MET:O	2:F:382:ILE:HG13	2.18	0.43
2:I:441:MET:HE1	2:I:559:ILE:HB	2.00	0.43
2:I:377:SER:CB	2:I:379:PRO:HD2	2.48	0.43
2:L:399:LEU:CD1	2:L:409:LEU:HD22	2.45	0.43
2:C:559:ILE:HG23	2:C:563:ASP:CB	2.47	0.43
2:B:446:LEU:HB2	2:B:564:TRP:CZ2	2.53	0.43
2:L:385:ARG:NH1	2:L:450:LEU:O	2.51	0.43
2:I:489:ASP:CA	2:I:535:LEU:HD21	2.48	0.43
2:K:326:ALA:O	2:K:366:ARG:NH2	2.51	0.43
2:F:557:PHE:HD2	2:F:558:ASN:H	1.67	0.43
2:B:442:LEU:O	2:B:443:CYS:C	2.55	0.43
2:B:458:ALA:HB2	2:C:491:TYR:HB3	2.01	0.43
2:E:309:GLU:O	2:E:310:LYS:C	2.56	0.43
2:G:441:MET:C	2:G:441:MET:SD	2.96	0.43
2:L:412:PHE:O	2:L:415:ALA:HB3	2.18	0.43
2:L:568:PHE:O	2:L:572:TRP:HB2	2.17	0.43
2:B:432:ILE:HD12	2:B:541:THR:HG21	2.00	0.43
2:F:412:PHE:HA	2:F:542:PHE:CZ	2.54	0.43
2:H:497:ASP:HB3	2:H:499:TYR:CD2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:447:ILE:HG13	2:A:476:LEU:CB	2.48	0.43
2:K:362:ALA:O	2:K:365:VAL:N	2.50	0.43
2:A:548:CYS:O	2:A:549:THR:C	2.57	0.43
2:E:378:MET:N	2:E:379:PRO:CD	2.80	0.43
2:D:349:LEU:HA	2:D:354:GLN:NE2	2.34	0.43
2:I:465:TRP:CG	2:I:465:TRP:O	2.71	0.43
2:D:312:ASP:OD2	2:D:315:THR:OG1	2.29	0.43
2:K:401:PHE:HE2	2:K:544:PHE:CE2	2.36	0.43
2:K:518:LEU:HA	2:K:518:LEU:HD23	1.86	0.43
2:L:434:PRO:CG	2:L:437:THR:HG21	2.48	0.43
2:I:316:MET:HE2	2:I:361:CYS:HB2	2.01	0.43
2:A:328:GLU:CB	2:B:367:HIS:HE1	2.17	0.43
2:K:525:ASP:OD1	2:K:527:GLN:HB2	2.19	0.43
2:C:401:PHE:CE2	2:C:544:PHE:HE2	2.26	0.43
2:E:362:ALA:O	2:E:363:THR:C	2.56	0.43
2:A:505:ARG:HG3	2:A:509:ALA:O	2.18	0.43
2:E:456:SER:OG	2:F:502:SER:HB3	2.18	0.43
2:L:552:SER:O	2:L:553:GLY:O	2.37	0.43
2:G:475:ALA:HB3	2:G:518:LEU:CD2	2.48	0.43
2:H:460:HIS:C	2:H:462:SER:H	2.21	0.43
2:G:321:TYR:C	2:G:321:TYR:CD1	2.92	0.43
2:L:448:HIS:CG	2:L:449:PHE:N	2.86	0.43
2:L:353:SER:O	2:L:357:HIS:CD2	2.71	0.43
2:F:429:LEU:HB2	2:F:519:LEU:HD23	2.00	0.43
2:A:334:GLU:O	2:A:337:LEU:HB2	2.18	0.43
2:I:500:PRO:HA	2:I:513:ILE:O	2.18	0.43
2:H:362:ALA:O	2:H:363:THR:C	2.57	0.43
2:H:459:ASN:OD1	2:I:463:HIS:HB2	2.18	0.43
2:G:546:GLN:HA	2:G:547:PRO:HD3	1.77	0.43
2:H:566:SER:O	2:H:567:PHE:C	2.57	0.43
2:L:503:ILE:HG22	2:L:511:VAL:HG12	2.01	0.43
2:L:383:LYS:CG	2:L:384:ALA:N	2.82	0.43
2:F:366:ARG:HG3	2:F:367:HIS:N	2.33	0.43
2:A:437:THR:HB	2:A:544:PHE:HB3	2.01	0.43
2:F:418:LEU:N	2:F:418:LEU:CD1	2.80	0.43
2:G:348:PHE:CZ	2:G:354:GLN:HB3	2.54	0.43
2:E:505:ARG:NH1	2:E:511:VAL:CG2	2.82	0.43
2:F:368:TYR:O	2:F:371:ALA:N	2.51	0.43
2:K:431:PHE:CE1	2:K:442:LEU:HD23	2.53	0.43
2:L:330:LYS:O	2:L:331:ILE:C	2.55	0.43
2:D:553:GLY:O	2:D:554:GLU:C	2.57	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:318:GLN:O	2:K:319:TRP:C	2.57	0.43
2:B:477:VAL:O	2:B:520:VAL:HA	2.18	0.43
2:K:439:LYS:HE3	5:L:11:ADP:O2B	2.18	0.43
2:E:444:ASN:OD1	2:F:500:PRO:HD2	2.18	0.43
2:B:499:TYR:CB	2:B:500:PRO:HD2	2.48	0.43
2:I:316:MET:O	2:I:319:TRP:HB3	2.19	0.43
2:G:316:MET:HE2	2:G:361:CYS:HB2	1.99	0.43
2:A:376:LEU:HD22	2:A:376:LEU:H	1.83	0.43
2:B:409:LEU:HG	2:B:413:ILE:HD11	2.01	0.43
2:B:328:GLU:O	2:B:329:SER:C	2.57	0.43
2:C:482:HIS:CE1	2:C:524:ILE:HD13	2.54	0.43
2:H:371:ALA:O	2:H:375:ALA:HB2	2.19	0.43
2:I:541:THR:CG2	2:I:542:PHE:N	2.82	0.43
2:I:378:MET:N	2:I:379:PRO:CD	2.82	0.42
2:K:486:ARG:NH1	2:K:486:ARG:HB2	2.33	0.42
2:E:543:ARG:H	2:E:543:ARG:HG2	1.72	0.42
2:D:453:SER:H	2:D:472:THR:HG21	1.83	0.42
2:A:533:LEU:HD12	2:A:536:HIS:ND1	2.34	0.42
2:K:439:LYS:HB2	5:L:11:ADP:O3B	2.19	0.42
2:E:410:ILE:HG23	2:E:411:THR:N	2.33	0.42
2:H:486:ARG:CZ	2:H:486:ARG:HB2	2.49	0.42
2:L:440:SER:HB2	2:L:444:ASN:H	1.84	0.42
2:L:382:ILE:CG2	2:L:568:PHE:HD1	2.32	0.42
2:K:455:LEU:CD1	2:K:466:LEU:HD23	2.49	0.42
2:I:377:SER:OG	2:I:379:PRO:HD2	2.18	0.42
2:L:534:TYR:CD2	2:L:534:TYR:O	2.73	0.42
2:G:493:ARG:O	2:G:497:ASP:OD2	2.37	0.42
2:D:377:SER:CB	2:D:379:PRO:HD2	2.49	0.42
2:I:489:ASP:O	2:I:493:ARG:NE	2.44	0.42
2:D:366:ARG:O	2:D:367:HIS:C	2.56	0.42
2:E:462:SER:C	2:E:464:PHE:N	2.73	0.42
2:F:457:PHE:O	2:F:460:HIS:HB3	2.19	0.42
2:H:328:GLU:HB3	2:I:367:HIS:CE1	2.54	0.42
2:B:464:PHE:CE2	2:B:506:LYS:HG2	2.54	0.42
2:I:477:VAL:HG21	2:I:488:PHE:HZ	1.84	0.42
2:E:313:PHE:CE2	2:E:317:VAL:CG2	3.02	0.42
2:C:473:ARG:O	2:C:517:PRO:HD2	2.19	0.42
2:C:475:ALA:HB3	2:C:518:LEU:HD23	2.01	0.42
2:J:485:TRP:CE3	2:J:526:VAL:HG11	2.54	0.42
2:I:370:ARG:HH21	2:I:511:VAL:HG11	1.83	0.42
2:L:420:LEU:C	2:L:422:GLY:N	2.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:454:VAL:HG23	2:I:512:GLN:OE1	2.19	0.42
2:I:546:GLN:HA	2:I:547:PRO:HD3	1.85	0.42
2:I:395:TRP:CE2	2:I:570:ARG:NE	2.86	0.42
2:K:453:SER:HB3	2:K:472:THR:HG21	2.00	0.42
2:L:458:ALA:C	2:L:460:HIS:N	2.72	0.42
2:J:501:VAL:HG22	2:J:502:SER:N	2.34	0.42
2:I:335:TYR:CE2	2:I:345:ALA:HA	2.54	0.42
2:D:441:MET:CE	2:D:559:ILE:H	2.32	0.42
2:J:429:LEU:HB2	2:J:519:LEU:HD23	2.01	0.42
2:B:401:PHE:CE2	2:B:544:PHE:CE2	3.05	0.42
2:F:316:MET:HE2	2:F:361:CYS:HB2	2.01	0.42
2:I:395:TRP:H	2:I:566:SER:HB3	1.85	0.42
2:J:316:MET:HE1	2:J:357:HIS:HB3	2.02	0.42
2:A:441:MET:HG2	2:A:442:LEU:H	1.85	0.42
2:H:357:HIS:O	2:H:358:VAL:C	2.58	0.42
2:D:325:TYR:CZ	2:D:334:GLU:HG2	2.54	0.42
2:L:552:SER:O	2:L:553:GLY:C	2.57	0.42
2:D:417:LYS:HG3	2:D:575:LEU:O	2.19	0.42
2:E:328:GLU:O	2:E:329:SER:C	2.56	0.42
2:A:503:ILE:HG13	2:A:513:ILE:CG2	2.50	0.42
2:H:497:ASP:CG	2:H:538:ARG:HE	2.23	0.42
2:G:409:LEU:HA	2:G:409:LEU:HD12	1.86	0.42
1:N:1:DT:H72	1:N:2:DT:N3	2.28	0.42
2:F:366:ARG:O	2:F:367:HIS:C	2.57	0.42
2:I:335:TYR:O	2:I:338:ALA:N	2.53	0.42
2:J:447:ILE:HD13	2:J:447:ILE:HA	1.96	0.42
2:H:441:MET:CE	2:H:559:ILE:H	2.31	0.42
2:G:362:ALA:O	2:G:363:THR:C	2.58	0.42
2:F:313:PHE:O	2:F:315:THR:N	2.52	0.42
2:J:370:ARG:HG3	2:J:471:ASP:OD2	2.19	0.42
2:G:475:ALA:HB3	2:G:518:LEU:HD23	2.01	0.42
2:B:327:GLU:O	2:B:328:GLU:C	2.56	0.42
2:H:316:MET:HE2	2:H:361:CYS:HB2	2.01	0.42
2:H:427:ASN:CG	2:H:427:ASN:O	2.58	0.42
2:L:574:ARG:CB	2:L:574:ARG:NH1	2.83	0.42
2:A:460:HIS:O	2:A:463:HIS:HA	2.20	0.42
1:M:4:DT:H1'	1:M:5:DT:H5'	2.01	0.42
2:I:377:SER:O	2:I:378:MET:C	2.57	0.42
2:E:376:LEU:O	2:E:473:ARG:NH2	2.53	0.42
2:H:492:LEU:CD1	2:H:492:LEU:N	2.82	0.42
2:F:454:VAL:HG13	2:F:476:LEU:HD13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:513:ILE:CG1	2:K:514:LYS:H	2.33	0.42
2:K:505:ARG:CZ	2:K:511:VAL:CG2	2.98	0.42
2:F:533:LEU:HD12	2:F:536:HIS:ND1	2.35	0.42
2:E:373:THR:HG23	2:E:381:TYR:HE1	1.84	0.42
2:B:462:SER:C	2:B:464:PHE:H	2.22	0.42
2:H:552:SER:O	2:H:553:GLY:C	2.58	0.42
2:K:455:LEU:HD21	2:K:475:ALA:CB	2.40	0.42
2:A:442:LEU:O	2:A:443:CYS:C	2.58	0.42
2:F:353:SER:O	2:F:357:HIS:CD2	2.72	0.42
2:F:441:MET:HG2	5:F:6:ADP:H1'	2.00	0.42
2:F:337:LEU:C	2:F:339:ALA:N	2.73	0.42
2:G:465:TRP:CE2	2:G:466:LEU:HG	2.54	0.42
2:D:487:TYR:CE1	2:D:491:TYR:HD1	2.38	0.42
2:L:405:GLN:HA	2:L:546:GLN:NE2	2.35	0.42
2:L:319:TRP:HH2	2:L:334:GLU:HB3	1.84	0.42
5:H:8:ADP:O3B	5:H:8:ADP:O2A	2.37	0.42
2:F:436:ASN:N	5:F:6:ADP:O2A	2.52	0.42
2:G:525:ASP:O	2:G:527:GLN:N	2.53	0.42
2:B:337:LEU:C	2:B:339:ALA:H	2.23	0.42
2:I:427:ASN:HD21	2:I:517:PRO:N	2.18	0.42
2:I:348:PHE:CZ	2:I:354:GLN:HB3	2.55	0.42
2:A:434:PRO:O	2:A:437:THR:HG23	2.20	0.42
2:F:504:ASP:OD1	2:F:505:ARG:N	2.53	0.42
2:L:385:ARG:O	2:L:388:LEU:HB2	2.20	0.42
2:J:441:MET:HE3	2:J:559:ILE:H	1.84	0.42
2:E:409:LEU:CD2	2:E:413:ILE:HD11	2.50	0.42
2:J:418:LEU:HD12	2:J:418:LEU:N	2.35	0.42
2:B:378:MET:O	2:B:382:ILE:HG13	2.20	0.42
2:K:418:LEU:HD12	2:K:418:LEU:H	1.85	0.42
2:K:401:PHE:CE2	2:K:544:PHE:CE2	3.08	0.42
2:K:482:HIS:CG	2:K:531:ARG:NH2	2.88	0.42
2:L:424:PRO:O	2:L:425:LYS:HB2	2.20	0.42
2:J:369:LEU:HD23	2:J:369:LEU:HA	1.79	0.42
2:I:478:ASP:HB3	2:J:494:ASN:HD21	1.85	0.42
2:H:498:GLY:O	2:H:514:LYS:HG3	2.19	0.42
2:F:351:THR:HG22	2:F:353:SER:N	2.26	0.42
2:H:378:MET:HG2	2:H:420:LEU:HB3	2.00	0.42
2:F:439:LYS:HE3	2:F:439:LYS:HB2	1.84	0.42
2:L:452:GLY:H	2:L:474:ALA:HB3	1.85	0.42
2:I:454:VAL:HG22	2:I:476:LEU:HD12	2.02	0.42
2:F:505:ARG:O	2:F:506:LYS:C	2.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:311:PHE:CZ	2:F:313:PHE:HA	2.55	0.42
2:I:463:HIS:C	2:I:465:TRP:H	2.24	0.42
2:A:568:PHE:O	2:A:569:VAL:C	2.58	0.42
2:A:568:PHE:O	2:A:572:TRP:N	2.52	0.42
2:G:518:LEU:HA	2:G:518:LEU:HD23	1.85	0.42
2:F:398:ILE:HD12	2:F:567:PHE:HB2	2.01	0.42
2:K:492:LEU:O	2:K:495:ALA:HB3	2.19	0.42
2:D:506:LYS:O	2:D:508:LYS:N	2.50	0.42
2:I:337:LEU:HA	2:I:337:LEU:HD23	1.92	0.42
2:C:398:ILE:HD12	2:C:567:PHE:HB2	2.02	0.42
2:L:446:LEU:HD11	2:L:559:ILE:HB	1.93	0.41
2:F:373:THR:C	2:F:375:ALA:N	2.71	0.41
2:A:351:THR:HG21	2:A:357:HIS:NE2	2.35	0.41
2:A:441:MET:CG	2:A:442:LEU:H	2.32	0.41
2:F:351:THR:HG21	2:F:357:HIS:CD2	2.55	0.41
2:B:529:GLU:HG3	2:B:531:ARG:HG2	2.01	0.41
2:B:531:ARG:HD3	2:K:486:ARG:NH2	2.26	0.41
2:F:453:SER:O	2:F:475:ALA:HA	2.20	0.41
2:K:482:HIS:CE1	2:K:524:ILE:HD13	2.55	0.41
2:H:435:PRO:O	2:H:436:ASN:HB2	2.19	0.41
2:A:481:THR:O	2:A:482:HIS:C	2.58	0.41
2:K:464:PHE:O	2:K:466:LEU:N	2.53	0.41
2:F:436:ASN:CA	5:F:6:ADP:O2A	2.66	0.41
2:A:519:LEU:HA	2:A:519:LEU:HD23	1.77	0.41
2:H:377:SER:O	2:H:378:MET:C	2.58	0.41
2:K:379:PRO:O	2:K:380:ALA:C	2.59	0.41
2:B:344:ASN:O	2:B:347:ALA:HB3	2.20	0.41
2:C:500:PRO:HA	2:C:513:ILE:O	2.21	0.41
2:E:373:THR:O	2:E:374:GLN:C	2.57	0.41
2:K:413:ILE:HD13	2:K:571:LEU:HD22	2.02	0.41
2:B:419:TRP:CD1	2:B:429:LEU:HG	2.56	0.41
2:G:495:ALA:O	2:G:498:GLY:N	2.41	0.41
2:J:316:MET:CE	2:J:361:CYS:HB2	2.50	0.41
1:M:3:DT:C4	1:M:4:DT:C4	3.08	0.41
2:C:372:GLU:O	2:C:376:LEU:HD13	2.20	0.41
2:J:502:SER:HA	2:J:511:VAL:O	2.20	0.41
2:J:556:PRO:HB2	2:J:557:PHE:CE1	2.56	0.41
2:A:473:ARG:O	2:A:517:PRO:HD2	2.19	0.41
2:G:490:THR:HG22	2:G:491:TYR:CE2	2.54	0.41
2:B:317:VAL:O	2:B:318:GLN:C	2.56	0.41
2:J:410:ILE:HG23	2:J:411:THR:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:565:LYS:O	2:I:569:VAL:HG23	2.20	0.41
2:L:461:LYS:HZ3	2:L:483:ALA:HB1	1.85	0.41
2:C:440:SER:O	2:C:441:MET:C	2.58	0.41
2:F:361:CYS:O	2:F:365:VAL:HG23	2.20	0.41
2:J:485:TRP:CD2	2:J:526:VAL:HG11	2.56	0.41
2:B:501:VAL:CG1	2:B:515:ALA:HB2	2.50	0.41
2:L:427:ASN:CG	2:L:427:ASN:O	2.57	0.41
2:F:450:LEU:HD23	2:F:450:LEU:HA	1.84	0.41
2:I:442:LEU:O	2:I:445:SER:OG	2.31	0.41
2:J:432:ILE:HD13	2:J:524:ILE:O	2.21	0.41
2:B:351:THR:HG21	2:B:357:HIS:NE2	2.35	0.41
2:F:401:PHE:HZ	2:F:438:GLY:HA3	1.84	0.41
2:I:354:GLN:O	2:I:355:ALA:C	2.58	0.41
2:D:489:ASP:O	2:D:493:ARG:NE	2.51	0.41
2:E:331:ILE:HD13	2:E:361:CYS:SG	2.60	0.41
2:I:409:LEU:HG	2:I:413:ILE:HD11	2.03	0.41
2:D:444:ASN:ND2	2:E:500:PRO:HD2	2.36	0.41
2:L:574:ARG:HB2	2:L:574:ARG:CZ	2.51	0.41
2:H:414:ASN:O	2:H:417:LYS:HB3	2.21	0.41
2:E:383:LYS:O	2:E:386:CYS:HB2	2.20	0.41
2:L:467:ALA:O	2:L:469:LEU:N	2.52	0.41
2:L:494:ASN:C	2:L:496:LEU:N	2.74	0.41
2:L:570:ARG:C	2:L:572:TRP:H	2.24	0.41
2:K:319:TRP:HH2	2:K:334:GLU:HB3	1.86	0.41
2:H:447:ILE:HG13	2:H:476:LEU:CB	2.47	0.41
2:A:370:ARG:HD2	2:A:471:ASP:OD2	2.20	0.41
2:G:316:MET:CE	2:G:361:CYS:HB2	2.51	0.41
2:K:476:LEU:O	2:K:476:LEU:HD13	2.20	0.41
2:G:363:THR:HG22	2:G:367:HIS:CD2	2.55	0.41
2:G:485:TRP:CE3	2:G:526:VAL:HG11	2.56	0.41
2:E:459:ASN:C	2:E:461:LYS:N	2.74	0.41
2:G:446:LEU:HD23	2:G:519:LEU:HD11	2.02	0.41
2:E:418:LEU:HD23	2:E:426:LYS:HD3	2.01	0.41
2:G:506:LYS:O	2:G:507:HIS:HB2	2.20	0.41
2:I:441:MET:HA	2:J:499:TYR:OH	2.21	0.41
2:A:353:SER:HB2	2:A:356:LYS:HB3	2.01	0.41
2:J:378:MET:HB3	2:J:379:PRO:CD	2.45	0.41
2:B:482:HIS:CE1	2:B:531:ARG:NH2	2.89	0.41
2:K:330:LYS:O	2:K:333:TYR:N	2.54	0.41
2:J:446:LEU:HB2	2:J:564:TRP:CZ2	2.56	0.41
2:C:332:ALA:HB1	2:D:364:MET:HE3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:363:THR:HG22	2:E:367:HIS:CD2	2.56	0.41
2:K:562:ALA:O	2:K:565:LYS:HB3	2.20	0.41
2:E:316:MET:HE1	2:E:357:HIS:HB3	2.03	0.41
2:J:459:ASN:O	2:J:461:LYS:N	2.54	0.41
2:E:568:PHE:O	2:E:572:TRP:N	2.54	0.41
2:J:423:ILE:HG23	2:J:424:PRO:HD2	2.02	0.41
2:F:309:GLU:O	2:F:310:LYS:O	2.39	0.41
2:H:432:ILE:HG13	2:H:541:THR:HG23	2.03	0.41
1:M:4:DT:C4'	2:E:507:HIS:CE1	3.00	0.41
2:H:319:TRP:CH2	2:H:334:GLU:HB3	2.54	0.41
2:L:525:ASP:C	2:L:525:ASP:OD1	2.59	0.41
2:B:418:LEU:H	2:B:418:LEU:CD1	2.32	0.41
2:A:427:ASN:CG	2:A:427:ASN:O	2.59	0.41
2:D:436:ASN:OD1	2:E:425:LYS:NZ	2.39	0.41
2:L:328:GLU:O	2:L:329:SER:C	2.59	0.41
2:E:339:ALA:HA	2:E:345:ALA:HB3	2.01	0.41
2:K:543:ARG:CG	2:K:543:ARG:HH11	2.33	0.41
5:L:11:ADP:O1B	5:L:11:ADP:O1A	2.39	0.41
2:E:441:MET:HE1	2:E:559:ILE:HB	2.03	0.41
2:L:437:THR:HG21	2:L:544:PHE:O	2.21	0.41
2:A:461:LYS:HD2	2:A:461:LYS:HA	1.81	0.41
2:B:497:ASP:OD1	2:B:538:ARG:HG2	2.20	0.41
2:D:432:ILE:HA	2:D:522:SER:O	2.21	0.41
2:C:439:LYS:CB	5:C:3:ADP:O2B	2.67	0.41
2:H:378:MET:N	2:H:379:PRO:CD	2.84	0.41
1:N:1:DT:C7	1:N:2:DT:N3	2.84	0.41
2:I:506:LYS:O	2:I:508:LYS:N	2.51	0.41
2:K:378:MET:N	2:K:379:PRO:HD3	2.36	0.41
2:B:418:LEU:HG	2:B:423:ILE:HD12	2.02	0.41
2:F:425:LYS:HE2	2:F:538:ARG:CZ	2.50	0.41
2:D:376:LEU:HD22	2:D:376:LEU:N	2.36	0.41
2:L:332:ALA:HB2	2:L:358:VAL:HG11	2.02	0.41
2:A:527:GLN:HA	2:A:536:HIS:HD2	1.86	0.41
2:F:546:GLN:HA	2:F:547:PRO:HD3	1.92	0.41
2:H:307:GLN:C	2:H:308:THR:O	2.59	0.41
2:K:311:PHE:CE1	2:K:348:PHE:HB2	2.55	0.41
2:H:481:THR:HG21	2:I:490:THR:O	2.21	0.41
2:J:459:ASN:C	2:J:461:LYS:N	2.74	0.41
2:L:573:GLY:C	2:L:575:LEU:H	2.23	0.41
2:G:492:LEU:N	2:G:492:LEU:CD1	2.83	0.41
2:J:335:TYR:C	2:J:337:LEU:N	2.75	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:482:HIS:ND1	2:D:524:ILE:HD13	2.35	0.41
2:H:457:PHE:CE1	2:H:460:HIS:CG	3.09	0.41
2:H:398:ILE:HD12	2:H:567:PHE:HB2	2.02	0.41
2:L:574:ARG:HH11	2:L:574:ARG:HB3	1.86	0.41
2:B:330:LYS:O	2:B:331:ILE:C	2.59	0.41
2:G:543:ARG:HG2	2:G:543:ARG:HH11	1.86	0.41
2:D:337:LEU:HD23	2:D:337:LEU:HA	1.88	0.41
2:L:395:TRP:N	2:L:566:SER:HB2	2.36	0.41
2:C:373:THR:O	2:C:376:LEU:N	2.52	0.41
2:D:497:ASP:HB3	2:D:499:TYR:HD2	1.86	0.41
2:L:432:ILE:HD13	2:L:525:ASP:CA	2.46	0.41
2:A:434:PRO:HD2	2:A:437:THR:HG21	2.03	0.41
2:G:351:THR:HG21	2:G:357:HIS:CD2	2.56	0.41
2:D:562:ALA:O	2:D:565:LYS:HB3	2.21	0.41
2:L:337:LEU:C	2:L:339:ALA:N	2.74	0.41
2:G:466:LEU:HD22	2:G:469:LEU:HD11	2.03	0.41
2:E:410:ILE:HG12	2:E:414:ASN:ND2	2.36	0.41
2:E:398:ILE:HD12	2:E:567:PHE:HB2	2.02	0.41
2:K:374:GLN:HB3	2:K:374:GLN:HE21	1.70	0.41
2:E:513:ILE:HA	2:E:513:ILE:HD12	1.88	0.41
2:H:541:THR:C	2:H:542:PHE:HD2	2.24	0.40
5:A:1:ADP:N7	2:B:424:PRO:HG2	2.36	0.40
2:H:478:ASP:CB	2:I:494:ASN:HD21	2.34	0.40
2:J:556:PRO:HB2	2:J:557:PHE:CD1	2.56	0.40
2:K:364:MET:O	2:K:367:HIS:HB2	2.21	0.40
2:D:372:GLU:O	2:D:376:LEU:CD2	2.68	0.40
2:F:531:ARG:NH1	2:K:404:TYR:HE1	2.18	0.40
2:J:425:LYS:HE2	2:J:538:ARG:NH1	2.37	0.40
2:C:441:MET:SD	2:C:441:MET:C	3.00	0.40
2:H:409:LEU:HG	2:H:413:ILE:CD1	2.51	0.40
2:E:550:ASP:CB	2:E:556:PRO:HD3	2.51	0.40
2:H:457:PHE:CE1	2:H:460:HIS:ND1	2.89	0.40
2:G:401:PHE:HE2	2:G:544:PHE:CE2	2.39	0.40
2:G:565:LYS:O	2:G:569:VAL:HG23	2.21	0.40
2:L:408:GLU:H	2:L:408:GLU:HG2	1.37	0.40
2:D:466:LEU:HB3	2:D:469:LEU:HD12	2.03	0.40
1:N:3:DT:H3'	2:I:464:PHE:CE2	2.51	0.40
2:G:501:VAL:HG22	2:G:502:SER:N	2.36	0.40
2:C:378:MET:N	2:C:379:PRO:CD	2.84	0.40
2:B:409:LEU:O	2:B:410:ILE:C	2.60	0.40
2:E:456:SER:HB2	2:F:502:SER:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:381:TYR:OH	2:F:450:LEU:O	2.34	0.40
2:I:401:PHE:HE2	2:I:544:PHE:CE2	2.40	0.40
2:F:466:LEU:HD23	2:F:466:LEU:HA	1.83	0.40
2:G:559:ILE:H	2:G:559:ILE:HG12	1.65	0.40
2:L:450:LEU:HA	2:L:450:LEU:HD23	1.96	0.40
2:L:327:GLU:O	2:L:328:GLU:C	2.59	0.40
2:J:490:THR:HG22	2:J:491:TYR:CD2	2.57	0.40
2:E:447:ILE:HG13	2:E:476:LEU:CB	2.51	0.40
2:H:434:PRO:O	2:H:437:THR:HG23	2.20	0.40
2:L:499:TYR:CB	2:L:500:PRO:HD2	2.52	0.40
2:K:459:ASN:OD1	2:L:464:PHE:CZ	2.74	0.40
2:K:331:ILE:HD13	2:K:361:CYS:SG	2.61	0.40
2:I:534:TYR:O	2:I:538:ARG:NH1	2.54	0.40
2:F:418:LEU:CD2	2:F:426:LYS:HG2	2.52	0.40
2:C:357:HIS:O	2:C:358:VAL:C	2.59	0.40
2:C:354:GLN:OE1	2:D:364:MET:HG2	2.22	0.40
2:I:485:TRP:CD2	2:I:526:VAL:CG1	3.05	0.40
2:G:364:MET:HE1	2:L:332:ALA:CB	2.50	0.40
2:C:513:ILE:CG1	2:C:514:LYS:N	2.84	0.40
2:G:337:LEU:C	2:G:339:ALA:H	2.25	0.40
2:C:552:SER:O	2:C:553:GLY:C	2.59	0.40
2:L:391:GLY:C	2:L:392:GLU:HG3	2.41	0.40
2:L:394:SER:O	2:L:397:SER:HB2	2.20	0.40
2:C:455:LEU:HD11	2:C:469:LEU:HD21	2.02	0.40
2:L:467:ALA:C	2:L:503:ILE:HG13	2.42	0.40
2:H:412:PHE:HA	2:H:542:PHE:CE1	2.57	0.40
2:J:505:ARG:NH1	2:J:511:VAL:HG23	2.36	0.40
2:J:345:ALA:O	2:J:348:PHE:HB3	2.22	0.40
2:H:457:PHE:CE2	2:H:484:CYS:HA	2.56	0.40
2:K:506:LYS:O	2:K:508:LYS:N	2.55	0.40
2:F:405:GLN:O	2:F:406:ASN:HB2	2.22	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
2	A	268/274 (98%)	212 (79%)	48 (18%)	8 (3%)	5 34
2	B	268/274 (98%)	221 (82%)	40 (15%)	7 (3%)	7 38
2	C	268/274 (98%)	232 (87%)	32 (12%)	4 (2%)	13 53
2	D	268/274 (98%)	224 (84%)	31 (12%)	13 (5%)	3 20
2	E	272/274 (99%)	229 (84%)	34 (12%)	9 (3%)	5 30
2	F	268/274 (98%)	215 (80%)	40 (15%)	13 (5%)	3 20
2	G	268/274 (98%)	225 (84%)	37 (14%)	6 (2%)	8 43
2	H	272/274 (99%)	227 (84%)	38 (14%)	7 (3%)	7 38
2	I	268/274 (98%)	220 (82%)	39 (15%)	9 (3%)	5 29
2	J	268/274 (98%)	218 (81%)	42 (16%)	8 (3%)	5 34
2	K	271/274 (99%)	219 (81%)	42 (16%)	10 (4%)	4 27
2	L	268/274 (98%)	180 (67%)	60 (22%)	28 (10%)	1 3
All	All	3227/3288 (98%)	2622 (81%)	483 (15%)	122 (4%)	4 26

All (122) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	376	LEU
2	A	549	THR
2	A	556	PRO
2	B	376	LEU
2	C	376	LEU
2	E	331	ILE
2	E	553	GLY
2	E	554	GLU
2	F	310	LYS
2	F	376	LEU
2	F	547	PRO
2	F	557	PHE
2	G	376	LEU
2	G	550	ASP
2	G	553	GLY
2	H	308	THR
2	H	376	LEU
2	J	376	LEU
2	J	510	ALA

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Mol	Chain	Res	Type
2	K	460	HIS
2	L	439	LYS
2	L	478	ASP
2	L	499	TYR
2	L	500	PRO
2	L	513	ILE
2	L	553	GLY
2	A	331	ILE
2	A	417	LYS
2	A	462	SER
2	B	457	PHE
2	B	553	GLY
2	C	374	GLN
2	D	399	LEU
2	D	400	THR
2	D	549	THR
2	E	551	GLU
2	F	441	MET
2	F	548	CYS
2	G	331	ILE
2	G	508	LYS
2	H	309	GLU
2	H	510	ALA
2	I	331	ILE
2	I	549	THR
2	J	375	ALA
2	K	331	ILE
2	K	548	CYS
2	L	375	ALA
2	L	440	SER
2	L	452	GLY
2	L	458	ALA
2	L	459	ASN
2	L	484	CYS
2	L	495	ALA
2	L	527	GLN
2	L	549	THR
2	A	508	LYS
2	B	550	ASP
2	D	463	HIS
2	E	310	LYS
2	E	463	HIS

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Mol	Chain	Res	Type
2	E	510	ALA
2	F	420	LEU
2	H	553	GLY
2	H	558	ASN
2	I	507	HIS
2	I	552	SER
2	I	554	GLU
2	J	331	ILE
2	J	549	THR
2	J	552	SER
2	K	507	HIS
2	K	556	PRO
2	L	393	GLY
2	L	466	LEU
2	L	536	HIS
2	L	573	GLY
2	C	469	LEU
2	D	331	ILE
2	D	355	ALA
2	D	424	PRO
2	D	550	ASP
2	D	552	SER
2	E	376	LEU
2	F	369	LEU
2	G	548	CYS
2	I	328	GLU
2	J	332	ALA
2	K	379	PRO
2	K	463	HIS
2	L	443	CYS
2	L	455	LEU
2	A	463	HIS
2	B	309	GLU
2	B	328	GLU
2	D	379	PRO
2	D	460	HIS
2	F	328	GLU
2	F	549	THR
2	I	336	ALA
2	I	460	HIS
2	J	424	PRO
2	K	465	TRP

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Mol	Chain	Res	Type
2	K	472	THR
2	L	359	LYS
2	L	390	THR
2	L	444	ASN
2	L	454	VAL
2	L	574	ARG
2	C	424	PRO
2	F	329	SER
2	H	379	PRO
2	I	553	GLY
2	K	510	ALA
2	L	467	ALA
2	D	547	PRO
2	E	379	PRO
2	F	314	GLY
2	F	331	ILE
2	D	553	GLY
2	L	331	ILE
2	B	331	ILE

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	
2	A	218/230 (95%)	210 (96%)	8 (4%)	41	78
2	B	218/230 (95%)	207 (95%)	11 (5%)	30	70
2	C	218/230 (95%)	207 (95%)	11 (5%)	30	70
2	D	218/230 (95%)	207 (95%)	11 (5%)	30	70
2	E	224/230 (97%)	208 (93%)	16 (7%)	18	56
2	F	218/230 (95%)	202 (93%)	16 (7%)	17	55
2	G	218/230 (95%)	205 (94%)	13 (6%)	24	63
2	H	224/230 (97%)	209 (93%)	15 (7%)	20	58
2	I	218/230 (95%)	208 (95%)	10 (5%)	33	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	J	218/230 (95%)	204 (94%)	14 (6%)	22 61
2	K	224/230 (97%)	208 (93%)	16 (7%)	18 56
2	L	218/230 (95%)	201 (92%)	17 (8%)	16 51
All	All	2634/2760 (95%)	2476 (94%)	158 (6%)	24 63

All (158) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	424	PRO
2	A	435	PRO
2	A	461	LYS
2	A	465	TRP
2	A	471	ASP
2	A	476	LEU
2	A	479	ASP
2	A	492	LEU
2	B	441	MET
2	B	473	ARG
2	B	476	LEU
2	B	479	ASP
2	B	489	ASP
2	B	492	LEU
2	B	494	ASN
2	B	501	VAL
2	B	511	VAL
2	B	523	ASN
2	B	540	GLN
2	C	367	HIS
2	C	424	PRO
2	C	441	MET
2	C	471	ASP
2	C	473	ARG
2	C	476	LEU
2	C	479	ASP
2	C	492	LEU
2	C	502	SER
2	C	523	ASN
2	C	540	GLN
2	D	364	MET
2	D	395	TRP
2	D	441	MET

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Mol	Chain	Res	Type
2	D	468	SER
2	D	471	ASP
2	D	473	ARG
2	D	476	LEU
2	D	479	ASP
2	D	523	ASN
2	D	526	VAL
2	D	540	GLN
2	E	318	GLN
2	E	441	MET
2	E	462	SER
2	E	468	SER
2	E	471	ASP
2	E	473	ARG
2	E	476	LEU
2	E	479	ASP
2	E	505	ARG
2	E	506	LYS
2	E	507	HIS
2	E	513	ILE
2	E	523	ASN
2	E	526	VAL
2	E	538	ARG
2	E	543	ARG
2	F	364	MET
2	F	376	LEU
2	F	441	MET
2	F	444	ASN
2	F	468	SER
2	F	471	ASP
2	F	476	LEU
2	F	479	ASP
2	F	492	LEU
2	F	512	GLN
2	F	523	ASN
2	F	526	VAL
2	F	538	ARG
2	F	540	GLN
2	F	543	ARG
2	F	557	PHE
2	G	318	GLN
2	G	364	MET

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Mol	Chain	Res	Type
2	G	372	GLU
2	G	414	ASN
2	G	441	MET
2	G	471	ASP
2	G	473	ARG
2	G	476	LEU
2	G	479	ASP
2	G	492	LEU
2	G	511	VAL
2	G	523	ASN
2	G	538	ARG
2	H	306	LEU
2	H	308	THR
2	H	318	GLN
2	H	441	MET
2	H	468	SER
2	H	471	ASP
2	H	473	ARG
2	H	476	LEU
2	H	479	ASP
2	H	492	LEU
2	H	513	ILE
2	H	517	PRO
2	H	523	ASN
2	H	526	VAL
2	H	540	GLN
2	I	364	MET
2	I	441	MET
2	I	463	HIS
2	I	468	SER
2	I	476	LEU
2	I	479	ASP
2	I	489	ASP
2	I	523	ASN
2	I	526	VAL
2	I	540	GLN
2	J	364	MET
2	J	441	MET
2	J	468	SER
2	J	471	ASP
2	J	473	ARG
2	J	476	LEU

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Mol	Chain	Res	Type
2	J	479	ASP
2	J	492	LEU
2	J	505	ARG
2	J	523	ASN
2	J	526	VAL
2	J	538	ARG
2	J	543	ARG
2	J	548	CYS
2	K	441	MET
2	K	455	LEU
2	K	459	ASN
2	K	468	SER
2	K	471	ASP
2	K	476	LEU
2	K	479	ASP
2	K	492	LEU
2	K	497	ASP
2	K	506	LYS
2	K	526	VAL
2	K	531	ARG
2	K	538	ARG
2	K	543	ARG
2	K	548	CYS
2	K	557	PHE
2	L	364	MET
2	L	408	GLU
2	L	441	MET
2	L	449	PHE
2	L	464	PHE
2	L	473	ARG
2	L	478	ASP
2	L	492	LEU
2	L	499	TYR
2	L	500	PRO
2	L	503	ILE
2	L	504	ASP
2	L	520	VAL
2	L	521	THR
2	L	533	LEU
2	L	564	TRP
2	L	569	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (76) such

sidechains are listed below:

Mol	Chain	Res	Type
2	A	427	ASN
2	A	444	ASN
2	A	512	GLN
2	B	318	GLN
2	B	367	HIS
2	B	436	ASN
2	B	494	ASN
2	B	523	ASN
2	B	546	GLN
2	C	318	GLN
2	C	374	GLN
2	C	414	ASN
2	C	427	ASN
2	C	436	ASN
2	C	494	ASN
2	C	523	ASN
2	D	318	GLN
2	D	354	GLN
2	D	374	GLN
2	D	444	ASN
2	D	494	ASN
2	D	507	HIS
2	D	523	ASN
2	E	318	GLN
2	E	367	HIS
2	E	414	ASN
2	E	427	ASN
2	E	507	HIS
2	E	523	ASN
2	F	318	GLN
2	F	367	HIS
2	F	414	ASN
2	F	459	ASN
2	F	507	HIS
2	F	523	ASN
2	G	318	GLN
2	G	367	HIS
2	G	427	ASN
2	G	444	ASN
2	G	512	GLN
2	G	523	ASN
2	H	318	GLN

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Mol	Chain	Res	Type
2	H	427	ASN
2	H	436	ASN
2	H	444	ASN
2	H	494	ASN
2	H	523	ASN
2	H	536	HIS
2	I	318	GLN
2	I	414	ASN
2	I	427	ASN
2	I	444	ASN
2	I	494	ASN
2	I	523	ASN
2	I	536	HIS
2	J	318	GLN
2	J	414	ASN
2	J	427	ASN
2	J	507	HIS
2	J	523	ASN
2	J	546	GLN
2	K	318	GLN
2	K	367	HIS
2	K	374	GLN
2	K	414	ASN
2	K	427	ASN
2	K	523	ASN
2	L	318	GLN
2	L	367	HIS
2	L	414	ASN
2	L	427	ASN
2	L	459	ASN
2	L	460	HIS
2	L	463	HIS
2	L	536	HIS
2	L	540	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 24 ligands modelled in this entry, 13 are monoatomic - leaving 11 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	$\#\|Z\| > 2$
5	ADP	A	1	3	22,29,29	1.45	2 (9%)	27,45,45	2.87	6 (22%)
5	ADP	B	2	3	22,29,29	1.43	3 (13%)	27,45,45	2.81	6 (22%)
5	ADP	C	3	3	22,29,29	1.44	3 (13%)	27,45,45	2.72	6 (22%)
5	ADP	D	4	3	22,29,29	1.37	2 (9%)	27,45,45	2.68	5 (18%)
5	ADP	E	5	3	22,29,29	1.36	2 (9%)	27,45,45	2.70	5 (18%)
5	ADP	F	6	-	22,29,29	1.24	2 (9%)	27,45,45	2.70	4 (14%)
5	ADP	G	7	3	22,29,29	1.49	2 (9%)	27,45,45	2.83	7 (25%)
5	ADP	H	8	3	22,29,29	1.34	2 (9%)	27,45,45	2.82	5 (18%)
5	ADP	J	9	3	22,29,29	1.39	2 (9%)	27,45,45	2.73	6 (22%)
5	ADP	K	10	3	22,29,29	1.37	2 (9%)	27,45,45	2.64	6 (22%)
5	ADP	L	11	3	22,29,29	1.94	4 (18%)	27,45,45	3.75	12 (44%)

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
5	ADP	A	1	3	-	0/12/32/32	0/3/3/3
5	ADP	B	2	3	-	0/12/32/32	0/3/3/3
5	ADP	C	3	3	-	0/12/32/32	0/3/3/3
5	ADP	D	4	3	-	0/12/32/32	0/3/3/3
5	ADP	E	5	3	-	0/12/32/32	0/3/3/3
5	ADP	F	6	-	-	0/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	ADP	G	7	3	-	0/12/32/32	0/3/3/3
5	ADP	H	8	3	-	0/12/32/32	0/3/3/3
5	ADP	J	9	3	-	0/12/32/32	0/3/3/3
5	ADP	K	10	3	-	0/12/32/32	0/3/3/3
5	ADP	L	11	3	-	0/12/32/32	0/3/3/3

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	11	ADP	C5'-C4'	-2.64	1.43	1.51
5	J	9	ADP	C8-N7	-2.25	1.30	1.34
5	A	1	ADP	C8-N7	-2.23	1.30	1.34
5	D	4	ADP	C8-N7	-2.21	1.30	1.34
5	H	8	ADP	C8-N7	-2.21	1.30	1.34
5	B	2	ADP	C8-N7	-2.18	1.30	1.34
5	G	7	ADP	C8-N7	-2.05	1.30	1.34
5	F	6	ADP	C8-N7	-2.05	1.30	1.34
5	C	3	ADP	C8-N7	-2.04	1.30	1.34
5	K	10	ADP	C8-N7	-2.03	1.30	1.34
5	E	5	ADP	C8-N7	-2.01	1.30	1.34
5	B	2	ADP	PB-O3B	2.18	1.62	1.54
5	C	3	ADP	PB-O3B	2.20	1.62	1.54
5	L	11	ADP	C2'-C3'	2.49	1.60	1.53
5	L	11	ADP	PB-O3B	2.88	1.65	1.54
5	F	6	ADP	O4'-C1'	3.77	1.46	1.41
5	K	10	ADP	O4'-C1'	4.27	1.46	1.41
5	H	8	ADP	O4'-C1'	4.28	1.46	1.41
5	E	5	ADP	O4'-C1'	4.44	1.46	1.41
5	D	4	ADP	O4'-C1'	4.48	1.46	1.41
5	J	9	ADP	O4'-C1'	4.76	1.47	1.41
5	C	3	ADP	O4'-C1'	4.79	1.47	1.41
5	B	2	ADP	O4'-C1'	4.81	1.47	1.41
5	A	1	ADP	O4'-C1'	4.90	1.47	1.41
5	G	7	ADP	O4'-C1'	5.27	1.47	1.41
5	L	11	ADP	O4'-C1'	6.54	1.49	1.41

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	G	7	ADP	N3-C2-N1	-10.41	120.92	128.89
5	E	5	ADP	N3-C2-N1	-10.18	121.10	128.89
5	L	11	ADP	C4'-O4'-C1'	-10.15	98.57	109.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	2	ADP	N3-C2-N1	-10.11	121.16	128.89
5	J	9	ADP	N3-C2-N1	-10.03	121.21	128.89
5	F	6	ADP	N3-C2-N1	-9.89	121.32	128.89
5	A	1	ADP	N3-C2-N1	-9.88	121.33	128.89
5	H	8	ADP	N3-C2-N1	-9.88	121.33	128.89
5	D	4	ADP	N3-C2-N1	-9.81	121.38	128.89
5	C	3	ADP	N3-C2-N1	-9.73	121.44	128.89
5	K	10	ADP	N3-C2-N1	-9.62	121.53	128.89
5	L	11	ADP	N3-C2-N1	-9.48	121.63	128.89
5	H	8	ADP	PA-O3A-PB	-8.20	105.19	132.67
5	F	6	ADP	PA-O3A-PB	-7.67	106.94	132.67
5	C	3	ADP	PA-O3A-PB	-7.67	106.96	132.67
5	D	4	ADP	PA-O3A-PB	-7.40	107.87	132.67
5	L	11	ADP	PA-O3A-PB	-7.22	108.46	132.67
5	B	2	ADP	PA-O3A-PB	-7.03	109.08	132.67
5	J	9	ADP	PA-O3A-PB	-7.03	109.09	132.67
5	G	7	ADP	PA-O3A-PB	-6.81	109.82	132.67
5	E	5	ADP	PA-O3A-PB	-6.62	110.48	132.67
5	K	10	ADP	PA-O3A-PB	-6.47	110.96	132.67
5	A	1	ADP	C2'-C1'-N9	-6.44	104.45	114.29
5	A	1	ADP	PA-O3A-PB	-6.31	111.51	132.67
5	B	2	ADP	C2'-C1'-N9	-5.43	105.99	114.29
5	E	5	ADP	C2'-C1'-N9	-4.86	106.86	114.29
5	L	11	ADP	C1'-N9-C4	-4.70	119.85	126.94
5	G	7	ADP	C2'-C1'-N9	-4.64	107.20	114.29
5	J	9	ADP	C2'-C1'-N9	-4.63	107.22	114.29
5	K	10	ADP	C2'-C1'-N9	-4.44	107.50	114.29
5	H	8	ADP	C2'-C1'-N9	-4.29	107.74	114.29
5	C	3	ADP	C2'-C1'-N9	-3.61	108.77	114.29
5	D	4	ADP	C2'-C1'-N9	-3.42	109.07	114.29
5	L	11	ADP	C4-C5-N7	-2.74	106.96	109.48
5	K	10	ADP	C4-C5-N7	-2.70	107.00	109.48
5	L	11	ADP	O2A-PA-O5'	-2.56	95.56	108.46
5	F	6	ADP	C4-C5-N7	-2.52	107.16	109.48
5	C	3	ADP	C4-C5-N7	-2.51	107.17	109.48
5	B	2	ADP	C4-C5-N7	-2.39	107.28	109.48
5	D	4	ADP	C4-C5-N7	-2.34	107.32	109.48
5	J	9	ADP	C4-C5-N7	-2.30	107.36	109.48
5	H	8	ADP	C4-C5-N7	-2.26	107.40	109.48
5	L	11	ADP	O3B-PB-O1B	-2.24	103.36	110.58
5	A	1	ADP	C4-C5-N7	-2.21	107.45	109.48
5	E	5	ADP	C4-C5-N7	-2.08	107.56	109.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	G	7	ADP	C4-C5-N7	-2.02	107.62	109.48
5	J	9	ADP	C2'-C3'-C4'	2.06	106.84	102.61
5	K	10	ADP	C2'-C3'-C4'	2.12	106.98	102.61
5	B	2	ADP	O4'-C1'-N9	2.13	112.55	108.10
5	E	5	ADP	C2'-C3'-C4'	2.15	107.03	102.61
5	C	3	ADP	C2'-C3'-C4'	2.19	107.12	102.61
5	K	10	ADP	O3A-PA-O5'	2.33	109.12	102.94
5	J	9	ADP	O3A-PA-O5'	2.38	109.25	102.94
5	G	7	ADP	O4'-C1'-N9	2.38	113.09	108.10
5	L	11	ADP	O5'-C5'-C4'	2.42	118.05	109.12
5	L	11	ADP	O4'-C4'-C5'	2.53	118.36	109.32
5	C	3	ADP	O3A-PA-O5'	2.55	109.70	102.94
5	G	7	ADP	O3A-PA-O5'	2.56	109.72	102.94
5	B	2	ADP	C2'-C3'-C4'	2.56	107.87	102.61
5	D	4	ADP	O3A-PA-O5'	2.58	109.79	102.94
5	A	1	ADP	C2'-C3'-C4'	2.65	108.06	102.61
5	G	7	ADP	C2'-C3'-C4'	2.75	108.27	102.61
5	H	8	ADP	O3A-PA-O5'	2.82	110.41	102.94
5	A	1	ADP	O4'-C1'-N9	2.86	114.09	108.10
5	L	11	ADP	C2'-C1'-N9	3.17	119.13	114.29
5	L	11	ADP	O3'-C3'-C4'	3.31	120.99	111.05
5	F	6	ADP	O3A-PA-O5'	3.40	111.96	102.94
5	L	11	ADP	O3A-PA-O5'	6.59	120.43	102.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 41 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1	ADP	4	0
5	B	2	ADP	5	0
5	C	3	ADP	4	0
5	D	4	ADP	2	0
5	E	5	ADP	2	0
5	F	6	ADP	11	0
5	G	7	ADP	3	0
5	H	8	ADP	5	0
5	J	9	ADP	1	0
5	K	10	ADP	1	0
5	L	11	ADP	3	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	M	6/13 (46%)	-0.62	0 100 100	60, 67, 70, 143	0
1	N	7/13 (53%)	-0.83	0 100 100	53, 64, 110, 140	0
2	A	270/274 (98%)	-0.51	2 (0%) 89 82	25, 55, 147, 188	0
2	B	270/274 (98%)	-0.54	1 (0%) 93 90	25, 49, 123, 195	0
2	C	270/274 (98%)	-0.21	10 (3%) 45 28	27, 67, 154, 200	0
2	D	270/274 (98%)	-0.42	3 (1%) 82 71	32, 69, 151, 194	0
2	E	274/274 (100%)	-0.48	0 100 100	25, 64, 131, 205	0
2	F	270/274 (98%)	-0.47	1 (0%) 93 90	26, 60, 131, 202	0
2	G	270/274 (98%)	-0.43	2 (0%) 89 82	25, 63, 129, 192	0
2	H	274/274 (100%)	-0.43	1 (0%) 93 90	26, 60, 135, 205	0
2	I	270/274 (98%)	-0.29	6 (2%) 65 49	25, 69, 153, 192	0
2	J	270/274 (98%)	-0.40	6 (2%) 65 49	27, 63, 136, 205	0
2	K	273/274 (99%)	-0.49	3 (1%) 82 71	25, 59, 150, 198	0
2	L	270/274 (98%)	0.12	15 (5%) 28 14	38, 119, 186, 205	0
All	All	3264/3314 (98%)	-0.38	50 (1%) 76 62	25, 64, 154, 205	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	550	ASP	5.5
2	J	308	THR	5.1
2	I	550	ASP	4.7
2	L	386	CYS	4.5
2	L	444	ASN	4.3
2	D	551	GLU	4.1
2	L	530	ASP	4.0
2	L	467	ALA	3.6

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Mol	Chain	Res	Type	RSRZ
2	H	551	GLU	3.6
2	F	552	SER	3.5
2	C	568	PHE	3.4
2	L	550	ASP	3.4
2	L	533	LEU	3.3
2	L	503	ILE	3.3
2	A	511	VAL	3.3
2	L	568	PHE	3.2
2	D	558	ASN	3.0
2	C	398	ILE	2.8
2	I	398	ILE	2.7
2	L	488	PHE	2.7
2	C	402	PHE	2.6
2	J	553	GLY	2.6
2	L	440	SER	2.6
2	G	554	GLU	2.5
2	G	553	GLY	2.5
2	C	575	LEU	2.5
2	I	558	ASN	2.5
2	K	333	TYR	2.5
2	B	550	ASP	2.4
2	C	311	PHE	2.4
2	J	548	CYS	2.4
2	L	435	PRO	2.4
2	K	460	HIS	2.3
2	K	553	GLY	2.3
2	I	575	LEU	2.3
2	L	498	GLY	2.2
2	C	574	ARG	2.2
2	C	564	TRP	2.2
2	A	553	GLY	2.2
2	I	564	TRP	2.2
2	L	339	ALA	2.2
2	J	348	PHE	2.2
2	J	311	PHE	2.1
2	C	308	THR	2.1
2	J	336	ALA	2.1
2	C	348	PHE	2.1
2	L	501	VAL	2.1
2	L	459	ASN	2.0
2	I	559	ILE	2.0
2	C	557	PHE	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

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
3	MG	J	30	1/1	0.99	0.34	4.41	36,36,36,36	0
5	ADP	B	2	27/27	0.93	0.23	2.00	55,69,88,88	0
4	CL	A	41	1/1	0.94	0.22	1.37	70,70,70,70	0
5	ADP	L	11	27/27	0.89	0.24	0.75	84,142,198,198	0
5	ADP	H	8	27/27	0.90	0.22	0.71	70,94,123,123	0
3	MG	B	22	1/1	0.95	0.17	0.61	25,25,25,25	0
5	ADP	E	5	27/27	0.92	0.19	0.46	77,105,195,195	10
3	MG	G	27	1/1	0.85	0.17	0.43	33,33,33,33	0
3	MG	A	21	1/1	0.97	0.18	0.26	25,25,25,25	0
5	ADP	F	6	27/27	0.91	0.19	0.24	65,130,198,198	10
5	ADP	G	7	27/27	0.92	0.18	0.22	58,70,90,90	0
5	ADP	A	1	27/27	0.93	0.17	0.19	31,65,66,66	0
5	ADP	K	10	27/27	0.96	0.22	0.14	67,74,133,133	10
5	ADP	D	4	27/27	0.86	0.22	0.13	81,119,162,162	10
3	MG	H	28	1/1	0.96	0.16	-0.00	25,25,25,25	0
5	ADP	C	3	27/27	0.91	0.18	-0.38	70,80,100,100	0
3	MG	I	29	1/1	0.70	0.16	-0.42	55,55,55,55	0
3	MG	D	24	1/1	0.97	0.14	-0.49	50,50,50,50	0
4	CL	B	42	1/1	0.88	0.14	-0.67	73,73,73,73	0
5	ADP	J	9	27/27	0.94	0.17	-0.91	89,126,182,182	10
4	CL	H	48	1/1	0.78	0.07	-1.90	80,80,80,80	0
3	MG	C	23	1/1	0.97	0.08	-5.85	25,25,25,25	0
3	MG	K	31	1/1	0.94	0.11	-	51,51,51,51	0
3	MG	E	25	1/1	0.82	0.19	-	30,30,30,30	0

6.5 Other polymers (i)

There are no such residues in this entry.