



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 07:06 AM EDT

PDB ID : 2GXA / pdb_00002gxa
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

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

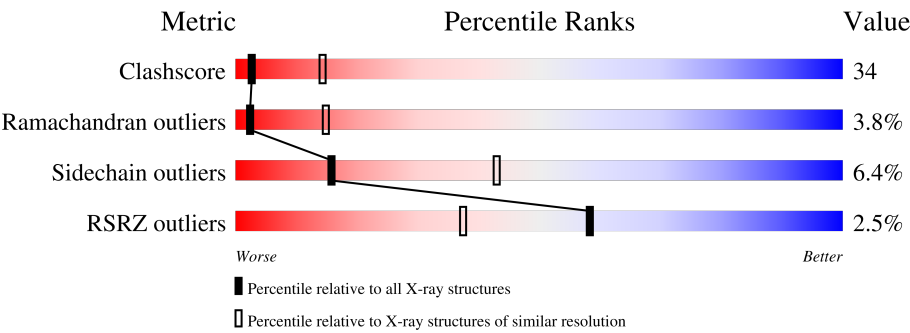
1 Overall quality at a glance i

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	190562	2486 (3.20-3.12)
Ramachandran outliers	187476	2405 (3.20-3.12)
Sidechain outliers	187428	2404 (3.20-3.12)
RSRZ outliers	180081	2361 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	M	13	15%31%54%
1	N	13	8%46%46%
2	A	274	% 45%44%9%..
2	B	274	44%47%7%..
2	C	274	3% 55%38%..
2	D	274	4% 46%45%7%. .

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Mol	Chain	Length	Quality of chain
2	E	274	
2	F	274	
2	G	274	
2	H	274	
2	I	274	
2	J	274	
2	K	274	
2	L	274	

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
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*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 (CCD ID: MG) (formula: Mg).

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

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

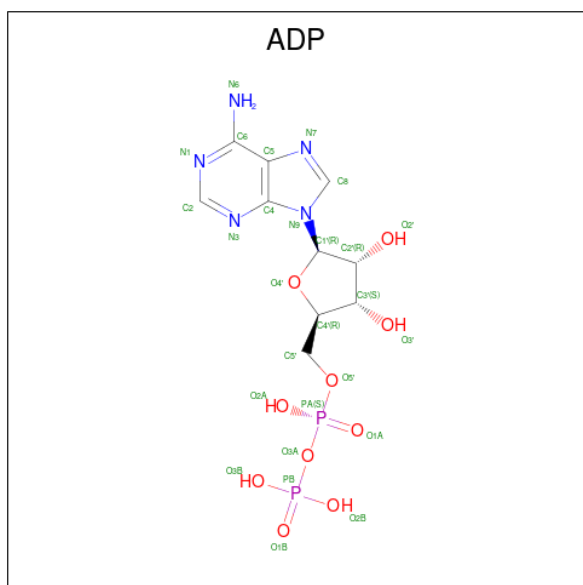
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Cl 1 1	0	0

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

- Molecule 5 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: 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	0	0
			27	10	5	10	2		
5	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	D	1	Total	C	N	O	P	10	0
			27	10	5	10	2		
5	E	1	Total	C	N	O	P	10	0
			27	10	5	10	2		
5	F	1	Total	C	N	O	P	10	0
			27	10	5	10	2		
5	G	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	H	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	J	1	Total	C	N	O	P	10	0
			27	10	5	10	2		

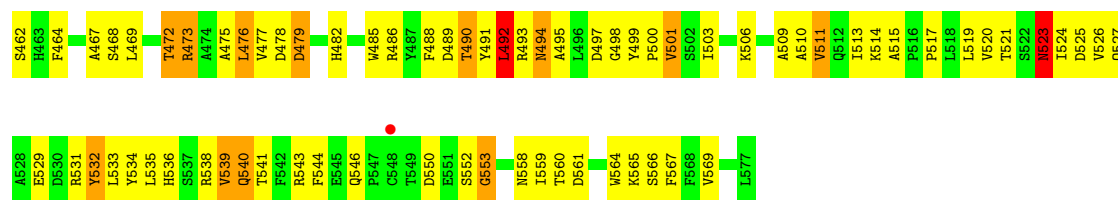
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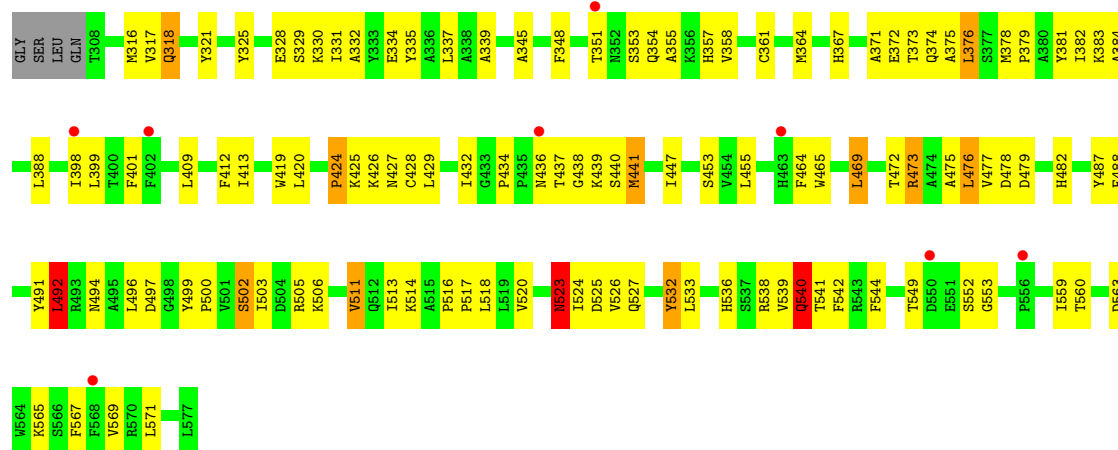
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	K	1	Total	C	N	O	P	10	0
			27	10	5	10	2		
5	L	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 6 is water.

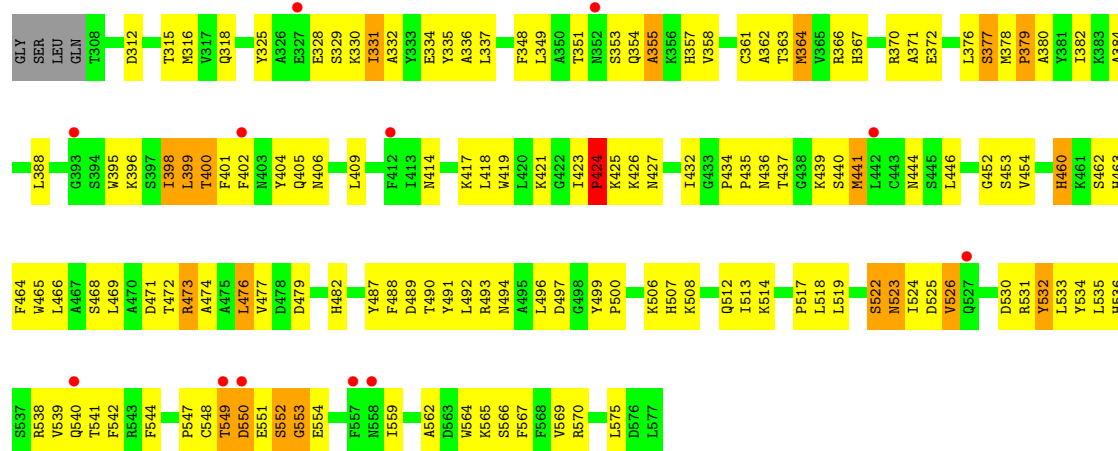
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	2	Total	O	0	0
			2	2		
6	B	3	Total	O	0	0
			3	3		
6	C	3	Total	O	0	0
			3	3		
6	D	1	Total	O	0	0
			1	1		
6	G	3	Total	O	0	0
			3	3		
6	H	2	Total	O	0	0
			2	2		
6	I	1	Total	O	0	0
			1	1		



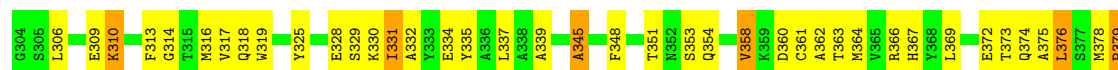
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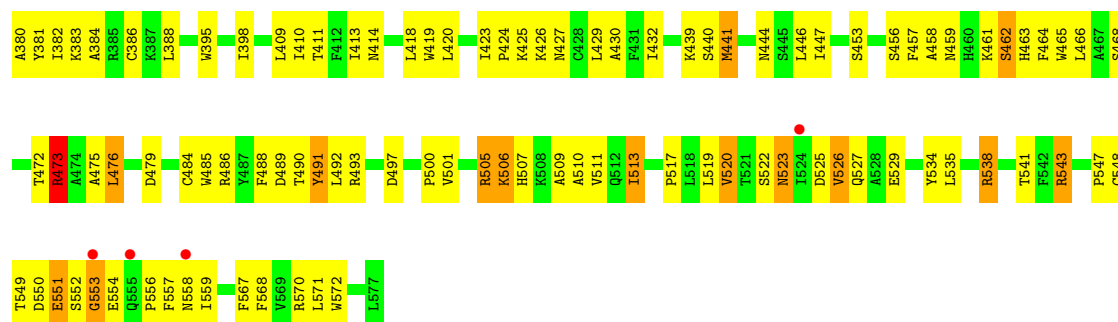


• Molecule 2: Replication protein E1

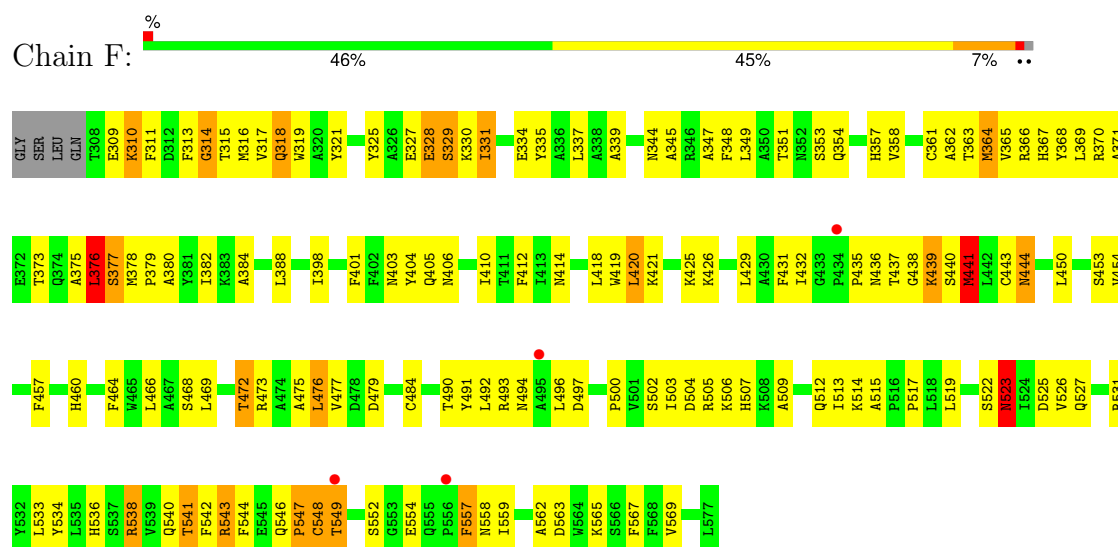


• Molecule 2: Replication protein E1

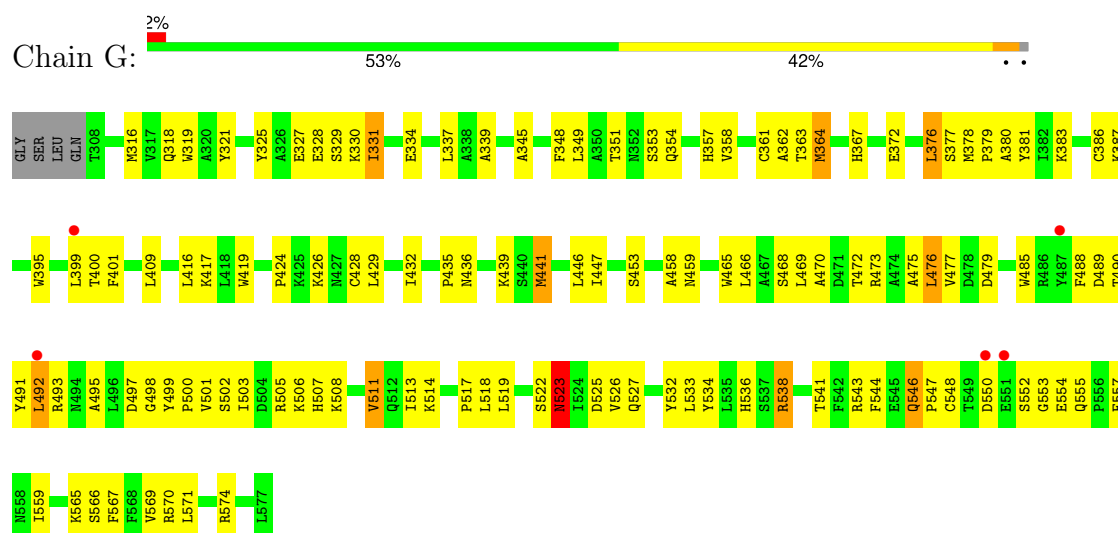




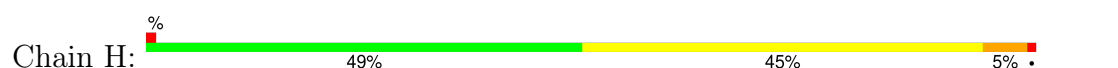
• Molecule 2: Replication protein E1

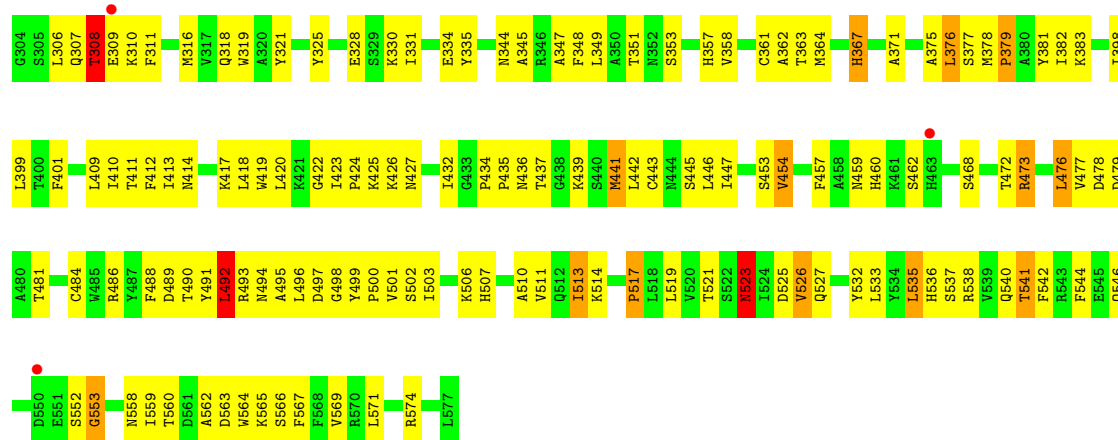


• Molecule 2: Replication protein E1

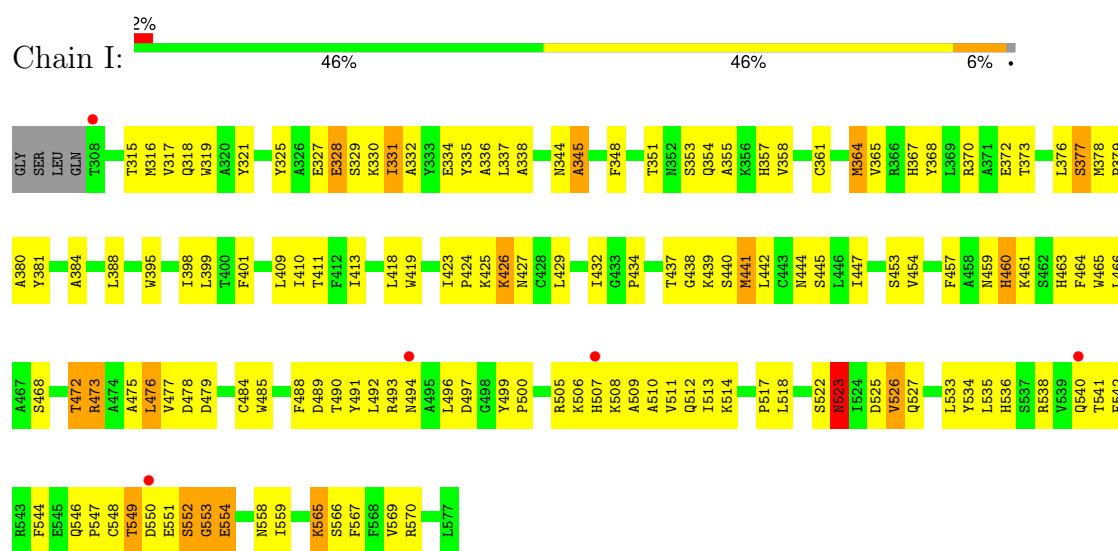


• Molecule 2: Replication protein E1

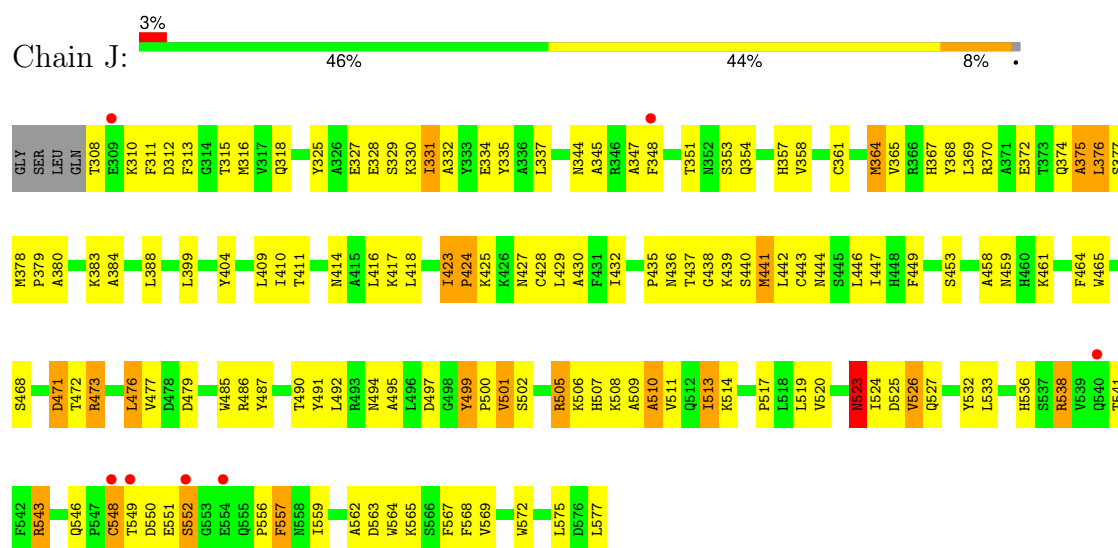




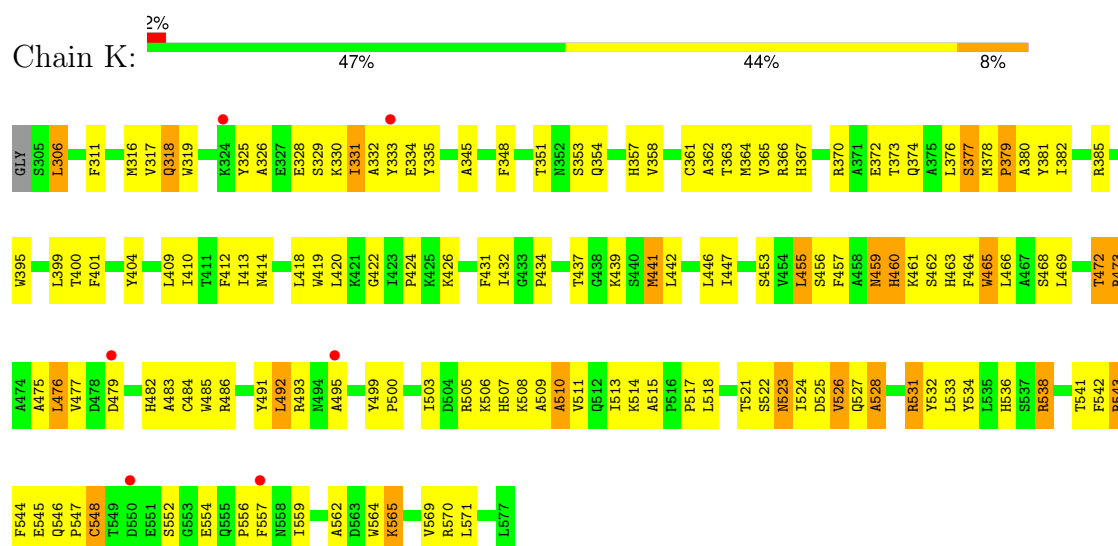
• Molecule 2: Replication protein E1



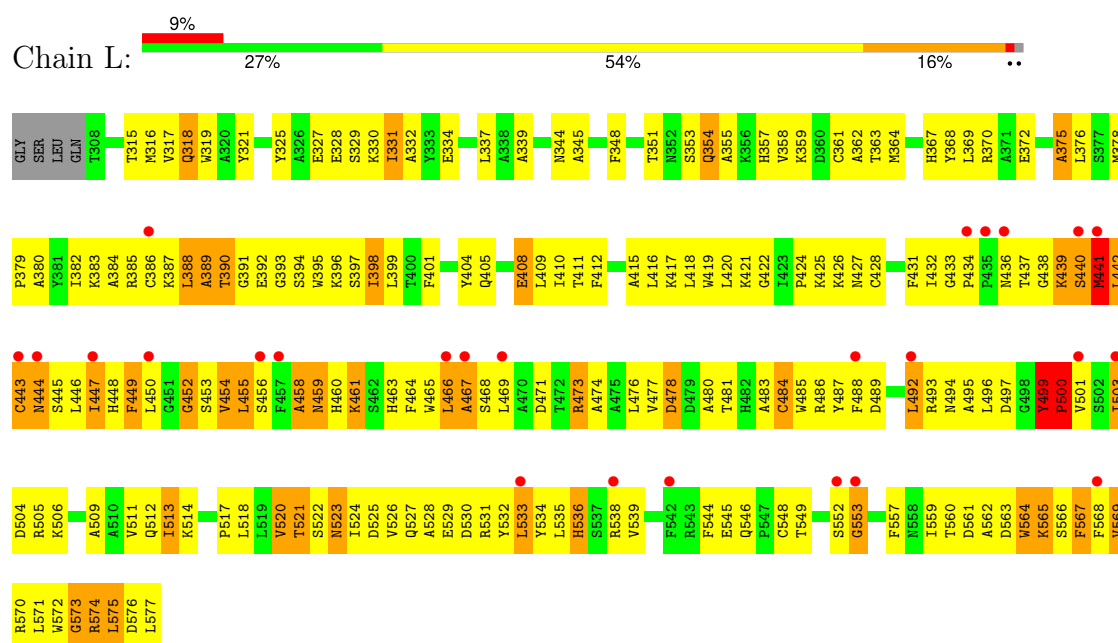
• Molecule 2: Replication protein E1



• Molecule 2: Replication protein E1



• Molecule 2: Replication protein E1



4 Data and refinement statistics

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 – 3.15	Depositor EDS
% Data completeness (in resolution range)	91.9 (44.65-3.15) 93.4 (44.65-3.15)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.33 (at 3.12Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.239 , 0.298 0.214 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	74.0	Xtriage
Anisotropy	0.151	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 47.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	M	0.52	0/132	1.12	0/200
1	N	0.50	0/154	0.98	0/234
2	A	0.86	3/2199 (0.1%)	1.24	25/2985 (0.8%)
2	B	0.63	1/2199 (0.0%)	1.06	14/2985 (0.5%)
2	C	0.53	0/2199	0.97	9/2985 (0.3%)
2	D	0.50	0/2199	0.96	7/2985 (0.2%)
2	E	0.53	0/2236	1.00	8/3033 (0.3%)
2	F	0.53	0/2199	0.98	8/2985 (0.3%)
2	G	0.52	0/2199	0.95	6/2985 (0.2%)
2	H	0.55	0/2236	1.00	11/3033 (0.4%)
2	I	0.50	0/2199	0.96	7/2985 (0.2%)
2	J	0.50	0/2199	0.97	7/2985 (0.2%)
2	K	0.55	0/2232	1.01	10/3028 (0.3%)
2	L	0.46	0/2199	1.12	21/2985 (0.7%)
All	All	0.56	4/26781 (0.0%)	1.02	133/36393 (0.4%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	460	HIS	CA-CB	-9.32	1.41	1.54
2	A	497	ASP	CB-CG	-9.07	1.29	1.52
2	A	497	ASP	CA-C	-5.81	1.44	1.52
2	B	539	VAL	CA-CB	-5.12	1.48	1.54

All (133) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	464	PHE	N-CA-C	-12.93	93.75	113.02
2	L	486	ARG	N-CA-C	-11.65	98.66	111.36
2	A	506	LYS	N-CA-C	10.91	122.86	110.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	500	PRO	CA-N-CD	-10.38	97.47	112.00
2	L	447	ILE	N-CA-C	-9.71	100.85	112.98
2	B	532	TYR	N-CA-C	-9.43	99.81	112.26
2	L	499	TYR	CA-C-N	9.39	131.58	119.84
2	L	499	TYR	C-N-CA	9.39	131.58	119.84
2	L	453	SER	N-CA-C	7.98	121.03	109.14
2	L	473	ARG	N-CA-C	7.97	123.22	113.17
2	L	499	TYR	N-CA-C	7.77	126.99	109.81
2	D	398	ILE	N-CA-C	-7.74	103.15	110.42
2	C	540	GLN	N-CA-C	-7.67	98.87	110.14
2	A	555	GLN	CA-C-N	7.63	129.38	119.84
2	A	555	GLN	C-N-CA	7.63	129.38	119.84
2	A	468	SER	N-CA-C	-7.47	102.81	112.23
2	A	523	ASN	N-CA-C	-7.43	104.02	113.23
2	G	532	TYR	N-CA-C	-7.43	104.17	112.57
2	H	541	THR	N-CA-C	7.24	121.34	109.24
2	L	441	MET	N-CA-C	-7.19	103.77	112.54
2	J	499	TYR	CA-C-N	6.94	126.92	119.78
2	J	499	TYR	C-N-CA	6.94	126.92	119.78
2	A	459	ASN	CB-CA-C	-6.93	101.24	111.77
2	E	558	ASN	N-CA-C	-6.88	97.36	109.06
2	I	377	SER	N-CA-C	-6.78	99.26	110.17
2	B	426	LYS	N-CA-C	-6.75	101.65	111.30
2	J	423	ILE	N-CA-C	6.67	114.36	108.63
2	C	426	LYS	N-CA-C	-6.62	102.84	111.71
2	A	377	SER	N-CA-C	-6.55	98.30	109.24
2	J	557	PHE	N-CA-C	6.54	119.07	108.41
2	H	523	ASN	N-CA-C	-6.52	105.33	113.28
2	F	403	ASN	N-CA-C	-6.40	104.22	111.07
2	E	423	ILE	CA-C-N	6.39	127.83	119.84
2	E	423	ILE	C-N-CA	6.39	127.83	119.84
2	F	523	ASN	N-CA-C	-6.38	105.50	113.28
2	C	523	ASN	N-CA-C	-6.37	105.27	113.16
2	L	481	THR	N-CA-C	-6.36	100.50	110.36
2	L	388	LEU	N-CA-C	6.31	119.82	110.48
2	A	548	CYS	N-CA-C	-6.30	105.72	113.41
2	A	542	PHE	N-CA-C	-6.29	99.46	109.59
2	K	523	ASN	N-CA-C	-6.28	105.62	113.28
2	F	541	THR	N-CA-C	6.25	119.13	109.07
2	A	497	ASP	CB-CG-OD1	-6.24	104.06	118.40
2	A	440	SER	N-CA-C	6.23	118.07	111.28
2	K	377	SER	N-CA-C	-6.21	101.02	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	461	LYS	N-CA-C	-6.20	105.68	113.18
2	K	515	ALA	CA-C-N	6.17	126.73	120.38
2	K	515	ALA	C-N-CA	6.17	126.73	120.38
2	K	456	SER	N-CA-C	-6.16	99.61	109.96
2	A	463	HIS	CA-C-N	-6.15	112.31	122.08
2	A	463	HIS	C-N-CA	-6.15	112.31	122.08
2	I	565	LYS	N-CA-C	-6.13	104.29	110.97
2	A	497	ASP	OD1-CG-OD2	6.08	137.50	122.90
2	H	492	LEU	N-CA-C	6.08	120.39	113.15
2	A	491	TYR	N-CA-C	6.07	120.70	113.12
2	C	492	LEU	N-CA-C	6.07	119.64	112.72
2	H	503	ILE	N-CA-C	6.05	116.64	108.17
2	A	465	TRP	N-CA-C	-6.03	106.58	112.97
2	D	532	TYR	N-CA-C	-6.02	104.31	112.26
2	F	377	SER	N-CA-C	-6.02	100.81	110.14
2	K	528	ALA	N-CA-C	5.96	117.57	111.14
2	H	426	LYS	N-CA-C	-5.95	103.80	113.19
2	G	426	LYS	N-CA-C	-5.91	103.61	112.54
2	D	539	VAL	N-CA-C	5.89	116.59	107.99
2	A	463	HIS	CB-CA-C	-5.88	98.73	110.42
2	I	523	ASN	N-CA-C	-5.82	106.14	113.18
2	D	426	LYS	N-CA-C	-5.82	103.76	112.54
2	G	523	ASN	N-CA-C	-5.82	106.19	113.28
2	L	389	ALA	N-CA-C	5.80	123.16	110.80
2	H	383	LYS	N-CA-C	-5.80	104.65	110.97
2	B	523	ASN	N-CA-C	-5.80	106.21	113.28
2	L	567	PHE	N-CA-C	-5.75	104.70	110.97
2	B	490	THR	N-CA-C	5.71	119.43	112.23
2	H	311	PHE	N-CA-C	5.70	118.46	109.96
2	E	473	ARG	N-CA-C	-5.68	105.93	112.92
2	K	372	GLU	N-CA-C	-5.67	104.74	111.03
2	H	546	GLN	N-CA-C	5.63	118.42	109.64
2	E	358	VAL	N-CA-C	-5.62	105.02	110.42
2	B	440	SER	N-CA-C	-5.61	105.06	111.07
2	B	521	THR	N-CA-C	-5.58	100.80	109.72
2	K	412	PHE	N-CA-C	-5.57	104.90	110.97
2	A	557	PHE	N-CA-C	5.57	118.99	110.20
2	L	523	ASN	N-CA-C	-5.56	106.17	113.17
2	A	497	ASP	CA-CB-CG	-5.55	107.05	112.60
2	C	511	VAL	CB-CA-C	-5.52	102.60	110.83
2	C	532	TYR	N-CA-C	-5.51	106.43	112.72
2	F	515	ALA	CA-C-N	5.50	126.05	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	515	ALA	C-N-CA	5.50	126.05	120.38
2	L	442	LEU	N-CA-C	-5.46	106.29	113.12
2	B	524	ILE	N-CA-C	5.44	116.14	108.36
2	B	492	LEU	N-CA-C	5.41	119.43	113.21
2	K	565	LYS	N-CA-C	-5.38	105.11	110.97
2	D	377	SER	N-CA-C	-5.36	101.53	110.17
2	B	546	GLN	CA-C-N	5.33	125.27	119.78
2	B	546	GLN	C-N-CA	5.33	125.27	119.78
2	J	486	ARG	N-CA-C	-5.32	105.38	111.07
2	C	428	CYS	N-CA-C	5.30	117.03	108.34
2	J	523	ASN	N-CA-C	-5.29	106.83	113.28
2	B	540	GLN	N-CA-C	-5.29	101.92	110.32
2	J	428	CYS	N-CA-C	5.27	117.67	108.76
2	I	345	ALA	N-CA-C	-5.27	105.43	111.07
2	B	472	THR	N-CA-C	5.26	117.47	110.53
2	L	509	ALA	N-CA-C	-5.25	103.96	110.41
2	D	490	THR	N-CA-C	5.24	119.59	112.04
2	L	354	GLN	N-CA-C	-5.23	105.47	111.07
2	A	472	THR	N-CA-C	5.21	118.00	110.28
2	C	516	PRO	CA-C-N	5.21	125.13	119.76
2	C	516	PRO	C-N-CA	5.21	125.13	119.76
2	H	521	THR	N-CA-C	-5.21	100.55	109.24
2	I	426	LYS	N-CA-C	-5.20	104.74	111.71
2	A	541	THR	N-CA-C	5.19	117.20	108.73
2	F	472	THR	N-CA-C	5.18	117.22	110.43
2	H	367	HIS	N-CA-C	-5.18	104.70	111.02
2	A	459	ASN	CA-C-N	-5.17	114.12	122.24
2	A	459	ASN	C-N-CA	-5.17	114.12	122.24
2	I	492	LEU	N-CA-C	5.17	118.45	112.97
2	G	546	GLN	CA-C-N	5.16	125.56	119.99
2	G	546	GLN	C-N-CA	5.16	125.56	119.99
2	G	522	SER	N-CA-C	5.14	116.66	108.79
2	E	345	ALA	N-CA-C	-5.12	105.59	111.07
2	L	499	TYR	C-N-CD	-5.11	104.06	125.00
2	B	455	LEU	N-CA-C	-5.10	102.93	110.48
2	F	439	LYS	N-CA-C	5.10	117.24	111.02
2	I	472	THR	N-CA-C	5.09	117.10	110.43
2	B	377	SER	N-CA-C	-5.08	101.83	109.85
2	H	535	LEU	N-CA-C	-5.07	106.79	113.17
2	L	456	SER	N-CA-C	-5.06	104.62	111.55
2	L	565	LYS	N-CA-C	-5.05	105.96	111.82
2	E	535	LEU	N-CA-C	5.05	116.79	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	466	LEU	N-CA-C	-5.05	105.17	113.50
2	K	521	THR	N-CA-C	-5.04	101.66	109.72
2	E	491	TYR	N-CA-C	5.02	119.28	112.04
2	D	522	SER	N-CA-C	5.01	116.14	108.52

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	16	0
1	N	141	0	85	19	0
2	A	2140	0	2078	172	0
2	B	2140	0	2078	149	0
2	C	2140	0	2078	107	0
2	D	2140	0	2078	131	0
2	E	2177	0	2124	125	0
2	F	2140	0	2078	145	0
2	G	2140	0	2078	109	0
2	H	2177	0	2125	137	0
2	I	2140	0	2077	144	0
2	J	2140	0	2078	128	0
2	K	2173	0	2121	153	0
2	L	2140	0	2078	296	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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	1	0	0	2	0
4	H	1	0	0	0	0
5	A	27	0	12	5	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	1741	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 34.

All (1741) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:390:THR:HG21	2:L:561:ASP:HB2	1.43	0.99
2:A:455:LEU:C	2:A:465:TRP:HZ3	1.71	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:CD2	2:F:376:LEU:H	1.79	0.96
2:K:455:LEU:N	2:K:455:LEU:HD23	1.80	0.95
2:L:444:ASN:HD22	2:L:521:THR:HG22	1.31	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:J:358:VAL:HG21	2:K:364:MET:HE1	1.51	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:A:424:PRO:O	2:A:425:LYS:HG2	1.67	0.92
2:L:418:LEU:H	2:L:418:LEU:HD12	1.33	0.92
2:L:431:PHE:HD1	2:L:440:SER:HG	0.99	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:C:539:VAL:HG12	2:C:540:GLN:O	1.71	0.91
2:L:446:LEU:CD1	2:L:559:ILE:HB	1.99	0.91
2:F:376:LEU:H	2:F:376:LEU:HD22	1.35	0.91
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:D:513:ILE:HD12	2:D:514:LYS:H	1.36	0.89
2:L:440:SER:HB2	2:L:443:CYS:HB2	1.55	0.89
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:533:LEU:HA	2:D:536:HIS:CE1	2.10	0.87
2:L:497:ASP:O	2:L:499:TYR:HD2	1.55	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:F:316:MET:HE3	2:F:361:CYS:HB2	1.59	0.85
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:H:439:LYS:HE3	5:H:8:ADP:O2B	1.78	0.84
2:L:454:VAL:CG1	2:L:455:LEU:H	1.91	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:A:455:LEU:C	2:A:465:TRP:CZ3	2.56	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:306:LEU:H	2:K:306:LEU:HD22	1.45	0.81
2:K:328:GLU:HB3	2:L:367:HIS:HE1	1.44	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
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:N	2:B:523:ASN:HD22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HD22	2:H:523:ASN:N	1.81	0.79
2:F:441:MET:HB2	5:F:6:ADP:O4'	1.81	0.79
2:L:476:LEU:HD13	2:L:477:VAL:N	1.98	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: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:442:LEU:O	2:L:446:LEU:CD1	2.31	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:L:485:TRP:CE3	2:L:526:VAL:HG11	2.19	0.77
2:F:410:ILE:HG12	2:F:414:ASN:ND2	1.99	0.77
2:B:316:MET:HE3	2:B:361:CYS:HB2	1.67	0.77
2:D:325:TYR:CE1	2:D:334:GLU:HG2	2.18	0.77
2:L:445:SER:O	2:L:446:LEU:HD23	1.85	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:G:316:MET:HE3	2:G:361:CYS:HB2	1.66	0.77
2:B:531:ARG:HD3	2:K:486:ARG:HH21	1.50	0.77
2:G:364:MET:HE1	2:L:358:VAL:HG21	1.66	0.77
2:H:325:TYR:CE1	2:H:334:GLU:HG2	2.20	0.77
2:L:446:LEU:HD13	2:L:559:ILE:HB	1.64	0.76
2:G:432:ILE:HD13	2:G:525:ASP:HA	1.65	0.76
2:D:523:ASN:HD22	2:D:523:ASN:N	1.82	0.76
2:I:523:ASN:HD22	2:I:523:ASN:N	1.80	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:439:LYS:HE3	5:K:10:ADP:O2B	1.85	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:K:316:MET:HE3	2:K:361:CYS:HB2	1.68	0.75
2:H:316:MET:HE3	2:H:361:CYS:HB2	1.69	0.75
2:G:399:LEU:HD13	2:G:409:LEU:HD22	1.68	0.75
2:E:325:TYR:CE1	2:E:334:GLU:HG2	2.21	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: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:E:316:MET:HE3	2:E:361:CYS:HB2	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:D:316:MET:HE3	2:D:361:CYS:HB2	1.68	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:E:358:VAL:HG21	2:F:364:MET:HE1	1.68	0.74
2:F:437:THR:OG1	2:F:439:LYS:HE2	1.88	0.74
2:F:438:GLY:HA2	5:F:6:ADP:H4'	1.69	0.74
2:C:523:ASN:HD22	2:C:523:ASN:N	1.85	0.73
2:L:316:MET:HE3	2:L:361:CYS:HB2	1.70	0.73
2:E:523:ASN:N	2:E:523:ASN:HD22	1.86	0.73
2:K:377:SER:OG	2:K:379:PRO:HD2	1.88	0.73
2:L:533:LEU:HA	2:L:536:HIS:CE1	2.23	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:A:316:MET:HE3	2:A:361:CYS:HB2	1.69	0.73
2:D:530:ASP:CG	2:G:533:LEU:HD21	2.14	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: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:J:505:ARG:NH1	2:J:505:ARG:HB2	2.05	0.72
2:L:476:LEU:HD22	2:L:477:VAL:H	1.52	0.72
2:J:358:VAL:CG2	2:K:364:MET:HE1	2.19	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:I:427:ASN:ND2	2:I:517:PRO:HA	2.04	0.72
2:L:494:ASN:HB2	2:L:501:VAL:HG22	1.70	0.72
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:HG2	2:B:370:ARG:HH11	1.55	0.71
2:B:494:ASN:HD22	2:B:494:ASN:N	1.88	0.71
2:L:447:ILE:CG1	2:L:564:TRP:CZ2	2.74	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: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:L:390:THR:HG21	2:L:561:ASP:CB	2.21	0.71
2:D:441:MET:HE1	2:D:559:ILE:HB	1.71	0.70
2:H:378:MET:HE2	2:H:473:ARG:HH12	1.56	0.70
2:K:373:THR:HA	2:K:376:LEU:HD23	1.72	0.70
2:E:486:ARG:HD3	2:L:528:ALA:O	1.90	0.70
2:L:437:THR:HG21	2:L:545:GLU:HA	1.70	0.70
1:M:3:DT:H5'	2:D:507:HIS:HD2	1.56	0.70
2:A:531:ARG:HH22	2:K:527:GLN:C	1.99	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:G:533:LEU:HA	2:G:536:HIS:ND1	2.06	0.70
2:K:455:LEU:HD23	2:K:455:LEU:H	1.52	0.70
2:L:485:TRP:CD2	2:L:526:VAL:HG11	2.27	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:L:483:ALA:C	2:L:485:TRP:H	1.99	0.70
2:L:496:LEU:HD13	2:L:538:ARG:HD2	1.73	0.70
2:A:455:LEU:CB	2:A:465:TRP:CZ3	2.74	0.69
2:C:432:ILE:CD1	2:C:525:ASP:HA	2.21	0.69
2:I:345:ALA:O	2:I:348:PHE:HB3	1.91	0.69
1:N:1:DT:H72	1:N:2:DT:H3	1.56	0.69
2:H:432:ILE:CD1	2:H:525:ASP:HA	2.21	0.69
2:A:534:TYR:CZ	2:A:538:ARG:CZ	2.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:L:512:GLN:O	2:L:513:ILE:CG1	2.34	0.69
2:L:512:GLN:C	2:L:513:ILE:HG13	2.18	0.69
2:A:325:TYR:CE1	2:A:334:GLU:HG2	2.27	0.69
2:B:499:TYR:HB3	2:B:500:PRO:HD2	1.74	0.69
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: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: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: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:401:PHE:HE2	2:A:544:PHE:CE2	2.11	0.68
2:L:398:ILE:HG22	2:L:399:LEU:N	2.06	0.68
2:A:418:LEU:H	2:A:418:LEU:CD1	2.06	0.68
2:A:456:SER:N	2:A:465:TRP:CZ3	2.61	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:E:351:THR:HG22	2:E:353:SER:H	1.58	0.68
2:F:440:SER:O	2:F:444:ASN:HB2	1.93	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:H	2:L:533:LEU:HD23	1.59	0.67
2:E:372:GLU:O	2:E:375:ALA:HB3	1.95	0.67
2:F:418:LEU:HD12	2:F:418:LEU:N	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:D:526:VAL:HG12	2:D:532:TYR:CD1	2.30	0.67
2:F:438:GLY:O	2:F:441:MET:HB3	1.94	0.67
2:A:382:ILE:HD11	2:A:420:LEU:HD22	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:F:476:LEU:HD22	2:F:477:VAL:N	2.10	0.66
2:J:328:GLU:HB3	2:K:367:HIS:HE1	1.60	0.66
2:D:427:ASN:OD1	2:D:517:PRO:HA	1.95	0.66
2:L:325:TYR:HE1	2:L:334:GLU:HG2	1.60	0.66
2:A:361:CYS:O	2:A:365:VAL:HG23	1.95	0.66
2:G:330:LYS:O	2:G:331:ILE:C	2.37	0.66
2:K:328:GLU:HB3	2:L:367:HIS:CE1	2.29	0.66
2:L:466:LEU:HG	2:L:467:ALA:N	2.10	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:H:376:LEU:HD23	2:H:381:TYR:CA	2.26	0.66
2:A:440:SER:O	2:A:444:ASN:HB2	1.95	0.65
2:A:457:PHE:N	2:A:465:TRP:CZ3	2.63	0.65
2:B:490:THR:HG22	2:B:491:TYR:CD2	2.31	0.65
2:H:358:VAL:HG21	2:I:364:MET:HE1	1.76	0.65
2:L:446:LEU:C	2:L:448:HIS:H	2.01	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:A:403:ASN:O	2:A:406:ASN:N	2.29	0.65
2:F:513:ILE:HG13	2:F:514:LYS:N	2.12	0.65
2:A:453:SER:HB3	2:A:472:THR:HG21	1.78	0.65
2:L:446:LEU:HB3	2:L:564:TRP:CZ3	2.31	0.65
2:K:325:TYR:CE1	2:K:334:GLU:HG2	2.32	0.65
2:L:437:THR:O	2:L:437:THR:HG22	1.96	0.65
2:D:460:HIS:HA	2:D:465:TRP:CD1	2.32	0.65
2:D:523:ASN:N	2:D:523:ASN:ND2	2.45	0.64
2:H:447:ILE:HG13	2:H:476:LEU:HB2	1.79	0.64
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:G:354:GLN:O	2:G:358:VAL:HG23	1.97	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:F:513:ILE:HG13	2:F:514:LYS:H	1.61	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:332:ALA:HB2	2:C:358:VAL:HG11	1.77	0.64
2:K:378:MET:O	2:K:382:ILE:HG13	1.97	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:H:316:MET:HE1	2:H:357:HIS:HB3	1.78	0.64
2:K:464:PHE:C	2:K:466:LEU:H	2.05	0.64
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:F:453:SER:HB3	2:F:472:THR:HG21	1.80	0.64
2:I:525:ASP:OD1	2:I:527:GLN:HB2	1.98	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:A:548:CYS:O	2:A:550:ASP:N	2.31	0.63
2:C:399:LEU:HD13	2:C:409:LEU:HD22	1.81	0.63
2:K:419:TRP:O	2:K:422:GLY:N	2.24	0.63
2:L:467:ALA:C	2:L:469:LEU:H	2.06	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:HD22	2:J:376:LEU:H	1.62	0.63
2:A:378:MET:HB3	2:A:379:PRO:HD3	1.81	0.62
2:A:497:ASP:N	2:A:497:ASP:OD1	2.28	0.62
2:C:316:MET:HE3	2:C:361:CYS:HB2	1.78	0.62
2:C:447:ILE:HG13	2:C:476:LEU:HB2	1.81	0.62
2:D:330:LYS:O	2:D:331:ILE:C	2.41	0.62
2:A:418:LEU:HD12	2:A:418:LEU:N	2.10	0.62
2:C:358:VAL:HG21	2:D:364:MET:HE1	1.81	0.62
2:G:490:THR:HG22	2:G:491:TYR:CD2	2.35	0.62
2:B:376:LEU:HD12	2:B:376:LEU:N	2.14	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:L:434:PRO:CG	2:L:437:THR:OG1	2.48	0.62
2:L:434:PRO:HD3	2:L:545:GLU:CD	2.24	0.62
2:L:436:ASN:C	2:L:438:GLY:H	2.05	0.62
2:B:376:LEU:HD12	2:B:376:LEU:H	1.63	0.62
2:J:432:ILE:HD12	2:J:541:THR:HG21	1.81	0.62
2:K:453:SER:CB	2:K:472:THR:HG21	2.30	0.62
2:G:447:ILE:HG13	2:G:476:LEU:HB2	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:503:ILE:O	2:G:511:VAL:HG23	2.00	0.62
2:I:332:ALA:HB2	2:I:358:VAL:HG11	1.81	0.62
2:C:476:LEU:HD22	2:C:476:LEU:C	2.25	0.62
2:D:328:GLU:HB3	2:E:367:HIS:CE1	2.35	0.62
2:F:469:LEU:HB2	2:F:503:ILE:HD13	1.80	0.62
2:L:390:THR:CG2	2:L:561:ASP:HB2	2.24	0.62
2:A:367:HIS:CE1	2:F:328:GLU:HB3	2.34	0.62
2:I:548:CYS:O	2:I:549:THR:C	2.41	0.62
2:J:505:ARG:HB2	2:J:505:ARG:HH11	1.63	0.62
1:M:3:DT:C1'	1:M:4:DT:H5''	2.30	0.62
2:E:441:MET:HE1	2:E:559:ILE:HB	1.81	0.62
2:F:401:PHE:O	2:F:404:TYR:HB3	2.00	0.62
2:H:424:PRO:HA	2:H:497:ASP:O	2.00	0.62
2:H:501:VAL:HG22	2:H:502:SER:N	2.15	0.62
2:K:462:SER:C	2:K:464:PHE:H	2.07	0.62
2:K:476:LEU:HD22	2:K:476:LEU:C	2.24	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:F:523:ASN:HD22	2:F:523:ASN:N	1.97	0.62
2:I:485:TRP:CE3	2:I:526:VAL:HG11	2.34	0.62
2:K:459:ASN:HB2	2:K:465:TRP:HB3	1.80	0.62
2:C:559:ILE:HG22	2:C:560:THR:N	2.14	0.61
2:I:513:ILE:HG13	2:I:514:LYS:N	2.15	0.61
2:L:434:PRO:CD	2:L:544:PHE:O	2.47	0.61
2:B:424:PRO:HA	2:B:497:ASP:O	2.00	0.61
2:K:455:LEU:N	2:K:455:LEU:CD2	2.55	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:L:438:GLY:HA2	2:L:441:MET:SD	2.39	0.61
2:G:476:LEU:C	2:G:476:LEU:HD22	2.26	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:I:330:LYS:O	2:I:331:ILE:C	2.44	0.61
1:N:3:DT:H3'	2:I:464:PHE:HE2	1.65	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: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:B:364:MET:O	2:B:367:HIS:HB2	2.00	0.61
2:A:364:MET:O	2:A:367:HIS:HB2	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:378:MET:HB3	2:E:379:PRO:HD3	1.82	0.61
2:F:497:ASP:OD2	2:F:538:ARG:NH1	2.33	0.61
2:K:419:TRP:CE2	2:K:517:PRO:HB3	2.36	0.61
2:D:435:PRO:O	2:D:436:ASN:HB2	2.01	0.60
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:A:456:SER:C	2:A:465:TRP:CZ3	2.79	0.60
2:A:465:TRP:CG	2:A:465:TRP:O	2.53	0.60
2:J:399:LEU:HD13	2:J:409:LEU:HD22	1.83	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:L:418:LEU:HD12	2:L:418:LEU:N	2.11	0.60
2:L:447:ILE:HG13	2:L:564:TRP:CZ2	2.36	0.60
2:L:467:ALA:C	2:L:469:LEU:N	2.55	0.60
2:B:376:LEU:H	2:B:376:LEU:CD1	2.15	0.60
2:G:351:THR:HG22	2:G:353:SER:H	1.65	0.60
2:G:476:LEU:HD22	2:G:477:VAL:N	2.16	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:E:330:LYS:O	2:E:331:ILE:C	2.43	0.60
2:J:476:LEU:HD22	2:J:476:LEU:C	2.26	0.60
2:F:354:GLN:O	2:F:358:VAL:HG23	2.02	0.60
2:K:533:LEU:HA	2:K:536:HIS:CE1	2.37	0.60
2:C:345:ALA:O	2:C:348:PHE:HB3	2.02	0.60
2:D:513:ILE:HD12	2:D:514:LYS:N	2.13	0.60
2:G:376:LEU:HD23	2:G:381:TYR:HA	1.82	0.60
2:H:523:ASN:N	2:H:523:ASN:ND2	2.46	0.60
2:L:421:LYS:HZ1	2:L:576:ASP:HB3	1.66	0.60
2:B:488:PHE:CE1	2:B:492:LEU:HD23	2.36	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:C:494:ASN:O	2:C:497:ASP:HB2	2.02	0.59
2:E:306:LEU:O	2:E:306:LEU:HD13	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:C:401:PHE:CE2	2:C:544:PHE:CE2	2.91	0.59
2:I:328:GLU:O	2:I:329:SER:C	2.43	0.59
2:I:351:THR:HG22	2:I:353:SER:H	1.67	0.59
2:I:438:GLY:O	2:I:441:MET:HB3	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:431:PHE:HD1	2:L:440:SER:OG	1.77	0.59
2:A:461:LYS:C	2:A:463:HIS:H	2.10	0.59
2:B:335:TYR:CE2	2:B:345:ALA:HA	2.37	0.59
2:B:441:MET:HE3	2:B:558:ASN:HA	1.84	0.59
2:H:441:MET:HE1	2:H:559:ILE:HG12	1.83	0.59
2:H:488:PHE:CE1	2:H:492:LEU:HD23	2.36	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:F:345:ALA:O	2:F:348:PHE:HB3	2.02	0.59
2:I:453:SER:O	2:I:475:ALA:HA	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:E:378:MET:O	2:E:382:ILE:HG13	2.03	0.59
2:F:418:LEU:HD12	2:F:418:LEU:H	1.65	0.59
2:J:441:MET:SD	2:J:441:MET:C	2.85	0.59
2:K:330:LYS:O	2:K:331:ILE:C	2.45	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:B:446:LEU:HD23	2:B:519:LEU:HD11	1.84	0.59
2:D:399:LEU:O	2:D:400:THR:C	2.45	0.59
2:J:316:MET:HE3	2:J:361:CYS:HB2	1.84	0.59
2:L:477:VAL:HB	2:L:520:VAL:HG13	1.84	0.59
2:L:494:ASN:O	2:L:496:LEU:N	2.30	0.59
2:D:348:PHE:CZ	2:D:354:GLN:HB3	2.38	0.59
2:D:432:ILE:HG23	2:D:522:SER:O	2.03	0.59
2:L:488:PHE:HB3	2:L:538:ARG:NH2	2.18	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
2:L:446:LEU:C	2:L:448:HIS:N	2.61	0.58
2:A:529:GLU:HG2	2:A:531:ARG:HE	1.68	0.58
2:H:525:ASP:OD1	2:H:527:GLN:HB2	2.03	0.58
2:H:526:VAL:HG12	2:H:532:TYR:CD1	2.37	0.58
2:L:466:LEU:HG	2:L:467:ALA:H	1.66	0.58
2:A:476:LEU:HD22	2:A:476:LEU:C	2.28	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:I:354:GLN:O	2:I:358:VAL:HG23	2.04	0.58
2:J:548:CYS:O	2:J:548:CYS:SG	2.61	0.58
2:K:441:MET:CE	2:K:559:ILE:H	2.16	0.58
2:J:505:ARG:NH1	2:J:509:ALA:O	2.30	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:494:ASN:C	2:L:496:LEU:H	2.11	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
5:H:8:ADP:H5'1	2:I:425:LYS:HD2	1.86	0.58
2:K:485:TRP:CE3	2:K:526:VAL:HG11	2.38	0.58
2:L:448:HIS:ND1	2:L:449:PHE:N	2.51	0.58
2:A:330:LYS:O	2:A:331:ILE:C	2.47	0.58
2:C:523:ASN:N	2:C:523:ASN:ND2	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:B:439:LYS:HB2	5:B:2:ADP:O2B	2.03	0.58
2:D:316:MET:CE	2:D:361:CYS:HB2	2.33	0.58
2:E:548:CYS:SG	2:E:557:PHE:HD1	2.27	0.58
2:F:476:LEU:HD22	2:F:476:LEU:C	2.28	0.58
2:K:523:ASN:HD22	2:K:523:ASN:N	2.01	0.58
2:L:385:ARG:HA	2:L:388:LEU:HD23	1.86	0.58
2:L:446:LEU:HA	2:L:448:HIS:ND1	2.18	0.58
2:A:432:ILE:CD1	2:A:525:ASP:HA	2.32	0.58
2:G:453:SER:N	2:G:472:THR:HG21	2.19	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: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:D:358:VAL:HG21	2:E:364:MET:HE1	1.86	0.57
2:D:531:ARG:HH12	2:L:524:ILE:HG12	1.69	0.57
2:I:500:PRO:HA	2:I:514:LYS:HA	1.86	0.57
2:A:447:ILE:HG13	2:A:476:LEU:HB2	1.86	0.57
2:G:513:ILE:HD12	2:G:514:LYS:H	1.68	0.57
2:H:376:LEU:HD23	2:H:381:TYR:N	2.19	0.57
2:I:489:ASP:HA	2:I:535:LEU:HD21	1.86	0.57
2:I:513:ILE:CG1	2:I:514:LYS:N	2.67	0.57
2:L:565:LYS:O	2:L:569:VAL:HG23	2.05	0.57
2:E:523:ASN:N	2:E:523:ASN:ND2	2.50	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:395:TRP:NE1	2:E:570:ARG:HD3	2.19	0.57
2:E:427:ASN:HD21	2:E:517:PRO:CA	2.13	0.57
2:F:316:MET:HE3	2:F:361:CYS:CB	2.34	0.57
2:E:465:TRP:NE1	2:E:466:LEU:HG	2.20	0.57
2:C:384:ALA:O	2:C:388:LEU:HD23	2.04	0.57
2:C:478:ASP:OD2	2:D:494:ASN:ND2	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:425:LYS:HG2	2:D:497:ASP:OD1	2.05	0.57
2:L:492:LEU:HD11	2:L:501:VAL:HG11	1.86	0.57
2:L:461:LYS:HE3	2:L:487:TYR:CD1	2.31	0.57
2:D:530:ASP:CG	2:G:533:LEU:CD2	2.78	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:458:ALA:HB2	2:H:491:TYR:HB3	1.86	0.56
2:I:441:MET:HE1	2:I:559:ILE:HB	1.87	0.56
2:K:469:LEU:HB2	2:K:503:ILE:HD13	1.87	0.56
2:L:433:GLY:O	2:L:523:ASN:HA	2.05	0.56
1:N:2:DT:H2''	1:N:3:DT:C6	2.41	0.56
2:A:377:SER:O	2:A:378:MET:C	2.48	0.56
2:B:441:MET:HE1	2:B:559:ILE:H	1.70	0.56
2:B:503:ILE:O	2:B:511:VAL:HG23	2.05	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:E:345:ALA:O	2:E:348:PHE:HB3	2.05	0.56
2:E:486:ARG:NE	2:L:528:ALA:HA	2.21	0.56
2:F:531:ARG:HH22	2:K:404:TYR:HD1	1.53	0.56
2:H:488:PHE:CE1	2:H:496:LEU:HD21	2.40	0.56
2:H:494:ASN:O	2:H:497:ASP:HB2	2.05	0.56
2:I:418:LEU:HD23	2:I:426:LYS:HD3	1.86	0.56
2:L:439:LYS:HG3	2:L:439:LYS:O	2.05	0.56
2:L:458:ALA:O	2:L:460:HIS:N	2.39	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
2:A:554:GLU:O	2:A:556:PRO:HD3	2.04	0.56
2:G:379:PRO:O	2:G:383:LYS:HB2	2.06	0.56
2:H:453:SER:HB3	2:H:472:THR:CG2	2.32	0.56
2:E:382:ILE:HD11	2:E:420:LEU:HD22	1.86	0.56
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:A:446:LEU:HD13	2:A:564:TRP:CH2	2.41	0.56
2:D:316:MET:HE3	2:D:361:CYS:CB	2.35	0.56
2:L:418:LEU:H	2:L:418:LEU:CD1	2.10	0.56
2:A:364:MET:HE1	2:F:358:VAL:HG21	1.88	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:345:ALA:O	2:A:348:PHE:HB3	2.06	0.56
2:H:494:ASN:HD22	2:H:494:ASN:N	2.02	0.56
2:I:410:ILE:HG23	2:I:411:THR:N	2.21	0.56
2:J:379:PRO:O	2:J:383:LYS:HB2	2.05	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:441:MET:SD	2:I:441:MET:C	2.89	0.56
2:I:473:ARG:O	2:I:517:PRO:HD2	2.05	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:CE3	2.84	0.56
2:B:418:LEU:N	2:B:418:LEU:CD1	2.69	0.56
2:H:478:ASP:HB3	2:I:494:ASN:HD21	1.70	0.56
1:M:2:DT:OP1	2:B:506:LYS:NZ	2.35	0.55
1:N:1:DT:H2"	1:N:2:DT:C6	2.41	0.55
2:B:424:PRO:O	2:B:425:LYS:HB2	2.04	0.55
2:D:476:LEU:HD22	2:D:476:LEU:C	2.31	0.55
2:J:430:ALA:HA	2:J:520:VAL:O	2.05	0.55
2:D:395:TRP:CD1	2:D:396:LYS:HG3	2.41	0.55
2:E:453:SER:HB3	2:E:472:THR:CG2	2.30	0.55
2:D:497:ASP:CG	2:D:538:ARG:HE	2.15	0.55
2:E:485:TRP:CD2	2:E:526:VAL:HG11	2.40	0.55
2:H:378:MET:HE2	2:H:473:ARG:NH1	2.21	0.55
2:B:489:ASP:HA	2:B:535:LEU:HD21	1.89	0.55
2:E:335:TYR:CE2	2:E:345:ALA:HA	2.40	0.55
2:L:382:ILE:O	2:L:386:CYS:SG	2.57	0.55
2:L:446:LEU:CD1	2:L:559:ILE:CB	2.80	0.55
2:F:315:THR:HB	2:F:344:ASN:ND2	2.20	0.55
2:G:441:MET:HE2	2:G:441:MET:O	2.06	0.55
2:K:453:SER:N	2:K:472:THR:HG21	2.21	0.55
2:A:428:CYS:SG	2:A:539:VAL:HG13	2.45	0.55
2:B:525:ASP:OD1	2:B:527:GLN:HB2	2.06	0.55
2:E:366:ARG:O	2:E:367:HIS:C	2.49	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
2:H:418:LEU:N	2:H:418:LEU:HD12	2.22	0.55
2:L:485:TRP:CZ3	2:L:526:VAL:HG21	2.42	0.55
2:L:562:ALA:O	2:L:565:LYS:HB3	2.06	0.55
2:D:496:LEU:HD23	2:D:518:LEU:HD12	1.89	0.55
2:A:461:LYS:C	2:A:463:HIS:N	2.64	0.55
2:B:358:VAL:HG21	2:C:364:MET:HE1	1.89	0.55
2:C:502:SER:C	2:C:503:ILE:HD13	2.32	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:313:PHE:O	2:F:314:GLY:C	2.50	0.55
2:F:376:LEU:HB3	2:F:380:ALA:HB3	1.88	0.55
2:I:316:MET:HE3	2:I:361:CYS:HB2	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:H:565:LYS:O	2:H:569:VAL:HG23	2.07	0.55
1:N:3:DT:H1'	2:J:507:HIS:CE1	2.41	0.55
2:A:358:VAL:HG21	2:B:364:MET:HE1	1.89	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
2:I:361:CYS:O	2:I:365:VAL:HG23	2.08	0.55
2:J:377:SER:O	2:J:378:MET:C	2.51	0.55
2:K:473:ARG:O	2:K:517:PRO:HD2	2.07	0.55
2:D:473:ARG:O	2:D:517:PRO:HD2	2.07	0.54
2:F:337:LEU:C	2:F:339:ALA:H	2.14	0.54
2:G:328:GLU:HB3	2:H:367:HIS:CE1	2.42	0.54
2:K:552:SER:C	2:K:554:GLU:H	2.14	0.54
2:L:569:VAL:HG12	2:L:570:ARG:N	2.21	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:J:427:ASN:ND2	2:J:517:PRO:HA	2.22	0.54
2:L:562:ALA:O	2:L:565:LYS:N	2.40	0.54
2:D:453:SER:HB3	2:D:472:THR:HG21	1.90	0.54
2:F:362:ALA:O	2:F:363:THR:C	2.50	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: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:H:478:ASP:HB3	2:I:494:ASN:ND2	2.22	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:K:447:ILE:HG13	2:K:476:LEU:HB2	1.90	0.54
2:K:541:THR:C	2:K:542:PHE:HD2	2.15	0.54
1:M:4:DT:C4'	2:E:507:HIS:HE1	2.20	0.54
2:D:332:ALA:HB2	2:D:358:VAL:HG11	1.89	0.54
2:F:378:MET:HB3	2:F:379:PRO:HD3	1.88	0.54
2:J:446:LEU:HD23	2:J:519:LEU:HD11	1.87	0.54
2:E:337:LEU:C	2:E:339:ALA:H	2.15	0.54
2:E:507:HIS:CE1	2:F:507:HIS:HD2	2.26	0.54
2:A:523:ASN:ND2	2:B:534:TYR:CZ	2.76	0.54
2:B:439:LYS:NZ	4:B:42:CL:CL	2.78	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:404:TYR:CE2	2:K:546:GLN:HB3	2.43	0.54
2:L:446:LEU:CB	2:L:564:TRP:CZ3	2.91	0.54
2:L:461:LYS:NZ	2:L:483:ALA:HB1	2.23	0.54
2:D:328:GLU:HB3	2:E:367:HIS:HE1	1.72	0.54
2:F:565:LYS:O	2:F:569:VAL:HG23	2.07	0.54
2:H:335:TYR:CE2	2:H:345:ALA:HA	2.43	0.54
2:H:559:ILE:HG22	2:H:560:THR:N	2.23	0.54
2:J:459:ASN:C	2:J:461:LYS:H	2.16	0.54
2:L:383:LYS:HG3	2:L:384:ALA:N	2.22	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:438:GLY:HA3	2:L:548:CYS:HB2	1.90	0.54
2:J:465:TRP:HZ2	2:J:487:TYR:CE2	2.26	0.54
2:L:380:ALA:O	2:L:383:LYS: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: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:L:546:GLN:OE1	2:L:546:GLN:N	2.42	0.53
2:B:529:GLU:HG2	2:B:531:ARG:HE	1.72	0.53
2:D:363:THR:HA	2:D:366:ARG:HD2	1.89	0.53
2:E:462:SER:C	2:E:464:PHE:H	2.17	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:H:308:THR:C	2:H:310:LYS:H	2.16	0.53
2:F:548:CYS:SG	2:F:549:THR:N	2.82	0.53
2:I:523:ASN:N	2:I:523:ASN:ND2	2.48	0.53
2:B:453:SER:HB3	2:B:472:THR:CG2	2.32	0.53
2:H:307:GLN:O	2:H:308:THR:O	2.25	0.53
2:H:453:SER:N	2:H:472:THR:HG21	2.23	0.53
2:K:362:ALA:O	2:K:363:THR:C	2.51	0.53
2:K:455:LEU:HD13	2:K:466:LEU:HD23	1.91	0.53
2:L:559:ILE:HG22	2:L:560:THR:O	2.08	0.53
2:A:403:ASN:O	2:A:404:TYR:C	2.51	0.53
2:K:335:TYR:CE2	2:K:345:ALA:HA	2.43	0.53
2:B:565:LYS:O	2:B:569:VAL:HG23	2.09	0.53
2:C:505:ARG:CZ	2:C:511:VAL:CG2	2.87	0.53
2:D:548:CYS:O	2:D:549:THR:C	2.51	0.53
2:L:467:ALA:O	2:L:503:ILE:HG13	2.08	0.53
2:A:335:TYR:CE2	2:A:345:ALA:HA	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:344:ASN:O	2:F:347:ALA:HB3	2.08	0.53
2:F:441:MET:HB2	5:F:6:ADP:C1'	2.38	0.53
2:L:401:PHE:HZ	2:L:405:GLN:HE21	1.56	0.53
2:C:328:GLU:O	2:C:329:SER:C	2.51	0.53
2:D:377:SER:H	2:D:380:ALA:HB3	1.74	0.53
2:F:525:ASP:OD1	2:F:527:GLN:HB2	2.08	0.53
2:F:547:PRO:O	2:F:548:CYS:HB3	2.09	0.53
2:H:501:VAL:HG22	2:H:502:SER:H	1.71	0.53
2:H:506:LYS:O	2:H:507:HIS:HB2	2.07	0.53
2:K:378:MET:N	2:K:379:PRO:CD	2.71	0.53
2:K:441:MET:HE3	2:K:559:ILE:H	1.73	0.53
2:L:434:PRO:HG2	2:L:437:THR:HG21	1.91	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:K:462:SER:C	2:K:464:PHE:N	2.67	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
1:N:3:DT:H2''	1:N:4:DT:C5'	2.39	0.52
2:G:386:CYS:O	2:G:387:LYS:C	2.53	0.52
2:I:513:ILE:CD1	2:I:514:LYS:H	2.22	0.52
2:J:375:ALA:O	2:J:376:LEU:O	2.27	0.52
2:K:447:ILE:HG13	2:K:476:LEU:CB	2.39	0.52
2:K:453:SER:O	2:K:475:ALA:HA	2.10	0.52
2:L:458:ALA:HB2	2:L:484:CYS:SG	2.49	0.52
2:L:489:ASP:CB	2:L:535:LEU:HD11	2.33	0.52
2:B:478:ASP:HB3	2:C:494:ASN:ND2	2.24	0.52
2:C:539:VAL:HG12	2:C:540:GLN:N	2.24	0.52
2:D:395:TRP:CZ2	2:D:570:ARG:NH1	2.75	0.52
2:D:530:ASP:OD1	2:G:533:LEU:HD21	2.09	0.52
2:E:432:ILE:HD12	2:E:541:THR:HG21	1.91	0.52
2:J:441:MET:HE1	2:J:559:ILE:HB	1.91	0.52
2:K:457:PHE:CD2	2:K:457:PHE:O	2.62	0.52
2:C:500:PRO:HA	2:C:514:LYS:HA	1.92	0.52
2:E:441:MET:HE2	2:E:441:MET:O	2.09	0.52
2:H:476:LEU:HD22	2:H:476:LEU:C	2.34	0.52
2:L:446:LEU:HD13	2:L:559:ILE:CB	2.38	0.52
2:A:328:GLU:O	2:A:329:SER:C	2.51	0.52
2:B:311:PHE:CE1	2:B:348:PHE:HB2	2.45	0.52
2:D:401:PHE:HE2	2:D:544:PHE:HE2	1.58	0.52
2:D:452:GLY:HA3	2:D:474:ALA:O	2.09	0.52
2:E:525:ASP:OD2	2:E:543:ARG:NH1	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:328:GLU:O	2:J:329:SER:C	2.53	0.52
1:M:3:DT:C2'	1:M:4:DT:H5''	2.39	0.52
2:A:376:LEU:HD12	2:A:380:ALA:HB1	1.92	0.52
2:A:442:LEU:HD12	2:A:559:ILE:HG13	1.90	0.52
2:F:453:SER:N	2:F:472:THR:HG21	2.25	0.52
2:G:424:PRO:HA	2:G:497:ASP:O	2.09	0.52
2:L:337:LEU:C	2:L:339:ALA:H	2.16	0.52
2:L:428:CYS:SG	2:L:539:VAL:HG22	2.50	0.52
2:L:445:SER:O	2:L:446:LEU:CD2	2.57	0.52
2:L:460:HIS:O	2:L:460:HIS:CG	2.63	0.52
2:B:513:ILE:HD12	2:B:514:LYS:H	1.75	0.52
2:L:494:ASN:HB3	2:L:499:TYR:HA	1.92	0.52
2:C:412:PHE:HA	2:C:542:PHE:CZ	2.45	0.52
2:D:439:LYS:HB2	5:D:4:ADP:O2B	2.09	0.52
2:E:506:LYS:O	2:E:507:HIS:HB2	2.09	0.52
2:H:401:PHE:HE2	2:H:544:PHE:HE2	1.57	0.52
2:I:490:THR:HG22	2:I:491:TYR:CD2	2.45	0.52
2:J:564:TRP:O	2:J:565:LYS:C	2.52	0.52
2:K:370:ARG:HG2	2:K:370:ARG:HH11	1.75	0.52
2:F:330:LYS:O	2:F:331:ILE:C	2.52	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:306:LEU:H	2:K:306:LEU:CD2	2.19	0.52
2:K:432:ILE:HA	2:K:522:SER:O	2.10	0.52
2:K:543:ARG:HG2	2:K:543:ARG:HH11	1.74	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: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: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:F:523:ASN:N	2:F:523:ASN:ND2	2.54	0.51
2:K:457:PHE:O	2:K:457:PHE:CG	2.63	0.51
2:L:399:LEU:HD13	2:L:409:LEU:CD2	2.41	0.51
2:A:485:TRP:CE3	2:A:526:VAL:HG11	2.45	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:F:494:ASN:C	2:F:496:LEU:N	2.65	0.51
2:L:434:PRO:HD2	2:L:437:THR:CG2	2.39	0.51
1:N:3:DT:C1'	1:N:4:DT:H5''	2.40	0.51
2:A:410:ILE:HG23	2:A:411:THR:N	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:441:MET:O	2:A:442:LEU:C	2.52	0.51
2:B:455:LEU:HD21	2:B:469:LEU:CD2	2.40	0.51
2:F:327:GLU:O	2:F:328:GLU:C	2.52	0.51
2:I:319:TRP:HH2	2:I:334:GLU:HB3	1.75	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:490:THR:HG22	2:B:491:TYR:CE2	2.45	0.51
5:B:2:ADP:H5'1	2:C:425:LYS:CD	2.40	0.51
2:E:453:SER:O	2:E:475:ALA:HA	2.10	0.51
2:F:328:GLU:O	2:F:329:SER:C	2.53	0.51
2:F:376:LEU:H	2:F:376:LEU:HD23	1.68	0.51
2:A:357:HIS:O	2:A:358:VAL:C	2.53	0.51
2:B:370:ARG:HG2	2:B:370:ARG:NH1	2.22	0.51
2:C:378:MET:HB3	2:C:379:PRO:HD3	1.92	0.51
2:D:454:VAL:HG22	2:D:476:LEU:HD12	1.92	0.51
2:F:321:TYR:CD1	2:F:321:TYR:C	2.89	0.51
2:H:419:TRP:CE2	2:H:517:PRO:HB3	2.45	0.51
2:H:571:LEU:CD2	2:H:574:ARG:HE	2.23	0.51
2:K:317:VAL:O	2:K:318:GLN:C	2.53	0.51
2:A:493:ARG:O	2:A:496:LEU:HB2	2.10	0.51
2:E:313:PHE:CE2	2:E:317:VAL:HG21	2.45	0.51
2:F:384:ALA:O	2:F:388:LEU:HD23	2.10	0.51
2:H:378:MET:CE	2:H:473:ARG:NH1	2.74	0.51
2:J:525:ASP:OD1	2:J:527:GLN:HB2	2.11	0.51
2:L:395:TRP:HB2	2:L:567:PHE:HA	1.93	0.51
2:E:354:GLN:O	2:E:358:VAL:HG23	2.11	0.51
2:E:490:THR:HG22	2:E:491:TYR:CD2	2.46	0.51
2:H:344:ASN:O	2:H:347:ALA:N	2.44	0.51
2:J:497:ASP:OD1	2:J:538:ARG:NH1	2.44	0.51
2:L:492:LEU:CD1	2:L:501:VAL:HG11	2.39	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:C:502:SER:O	2:C:503:ILE:HD13	2.11	0.51
2:D:362:ALA:O	2:D:366:ARG:HG2	2.11	0.51
2:J:374:GLN:OE1	2:J:374:GLN:HA	2.10	0.51
2:K:306:LEU:HD22	2:K:306:LEU:N	2.21	0.51
2:K:353:SER:O	2:K:357:HIS:CD2	2.64	0.51
2:L:321:TYR:C	2:L:321:TYR:CD1	2.88	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:F:431:PHE:CD2	2:F:443:CYS:SG	3.04	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:435:PRO:O	2:J:436:ASN:HB2	2.10	0.51
2:L:432:ILE:HG22	2:L:433:GLY:N	2.26	0.51
1:N:3:DT:C2'	1:N:4:DT:H5''	2.41	0.50
2:A:494:ASN:C	2:A:496:LEU:N	2.67	0.50
2:B:384:ALA:O	2:B:388:LEU:HD23	2.10	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:H:344:ASN:O	2:H:347:ALA:HB3	2.11	0.50
2:I:327:GLU:O	2:I:328:GLU:C	2.54	0.50
2:K:505:ARG:NE	2:K:511:VAL:HG23	2.26	0.50
2:C:438:GLY:O	2:C:441:MET:HB3	2.11	0.50
2:G:439:LYS:HB2	5:G:7:ADP:O2B	2.12	0.50
2:L:437:THR:HG23	2:L:546:GLN:N	2.26	0.50
2:L:483:ALA:C	2:L:485:TRP:N	2.63	0.50
1:N:4:DT:H1'	1:N:5:DT:O4'	2.10	0.50
2:G:364:MET:O	2:G:367:HIS:HB2	2.12	0.50
2:H:331:ILE:HD12	2:H:362:ALA:HB2	1.92	0.50
2:H:401:PHE:HE2	2:H:544:PHE:CE2	2.29	0.50
2:I:381:TYR:O	2:I:384:ALA:N	2.45	0.50
2:I:460:HIS:HA	2:I:465:TRP:CG	2.46	0.50
2:L:363:THR:HG22	2:L:367:HIS:CD2	2.46	0.50
2:A:461:LYS:O	2:A:463:HIS:N	2.44	0.50
2:E:316:MET:O	2:E:319:TRP:HB3	2.12	0.50
2:F:493:ARG:HD3	2:F:534:TYR:CE2	2.46	0.50
2:G:349:LEU:HA	2:G:354:GLN:HE21	1.76	0.50
2:J:312:ASP:OD2	2:J:315:THR:OG1	2.29	0.50
2:A:477:VAL:HG21	2:A:488:PHE:HZ	1.77	0.50
2:B:467:ALA:O	2:B:468:SER:C	2.53	0.50
2:I:434:PRO:O	2:I:437:THR:HG23	2.12	0.50
2:K:464:PHE:C	2:K:466:LEU:N	2.66	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:J:513:ILE:HG23	2:J:514:LYS:N	2.25	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:L:351:THR:HG21	2:L:357:HIS:CD2	2.47	0.50
2:L:362:ALA:O	2:L:363:THR:C	2.54	0.50
2:L:560:THR:HG1	2:L:563:ASP:CG	2.20	0.50
2:F:438:GLY:CA	5:F:6:ADP:H4'	2.40	0.50
2:G:513:ILE:CD1	2:G:514:LYS:H	2.24	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:308:THR:O	2:H:310:LYS:N	2.45	0.50
2:H:511:VAL:HG12	2:H:513:ILE:HG22	1.93	0.50
2:I:427:ASN:HD21	2:I:517:PRO:HA	1.76	0.50
2:I:494:ASN:O	2:I:497:ASP:HB2	2.12	0.50
2:K:432:ILE:HD12	2:K:541:THR:HG21	1.94	0.50
2:K:441:MET:HE1	2:K:559:ILE:HG12	1.94	0.50
2:L:572:TRP:C	2:L:572:TRP:CD1	2.90	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:J:418:LEU:HD12	2:J:418:LEU:H	1.75	0.50
2:J:551:GLU:O	2:J:552:SER:C	2.55	0.50
2:K:446:LEU:HB2	2:K:564:TRP:CZ2	2.47	0.50
2:L:434:PRO:HG2	2:L:437:THR:CG2	2.42	0.50
2:B:492:LEU:HD13	2:B:492:LEU:N	2.27	0.49
2:C:373:THR:C	2:C:375:ALA:N	2.70	0.49
2:D:378:MET:O	2:D:382:ILE:HG13	2.12	0.49
2:E:363:THR:O	2:E:367:HIS:CD2	2.65	0.49
2:G:485:TRP:CD2	2:G:526:VAL:HG11	2.47	0.49
2:J:414:ASN:O	2:J:418:LEU:HD13	2.11	0.49
2:K:513:ILE:CG1	2:K:514:LYS:N	2.75	0.49
2:G:358:VAL:HG21	2:H:364:MET:HE1	1.93	0.49
2:G:502:SER:O	2:G:503:ILE:HD13	2.12	0.49
2:G:523:ASN:N	2:G:523:ASN:ND2	2.60	0.49
2:L:416:LEU:HD12	2:L:419:TRP:CE3	2.47	0.49
2:L:418:LEU:HD22	2:L:426:LYS:HD3	1.93	0.49
2:L:420:LEU:C	2:L:422:GLY:H	2.20	0.49
2:B:479:ASP:OD2	2:C:538:ARG:NH2	2.45	0.49
2:C:376:LEU:HD23	2:C:381:TYR:CA	2.37	0.49
2:D:489:ASP:CA	2:D:535:LEU:HD21	2.40	0.49
2:E:550:ASP:O	2:E:551:GLU:C	2.55	0.49
2:G:499:TYR:HB3	2:G:500:PRO:HD2	1.94	0.49
2:I:441:MET:SD	2:I:442:LEU:N	2.85	0.49
2:I:553:GLY:O	2:I:554:GLU:C	2.54	0.49
2:J:509:ALA:O	2:J:510:ALA:O	2.31	0.49
2:K:526:VAL:HG12	2:K:532:TYR:CD1	2.46	0.49
2:B:492:LEU:N	2:B:492:LEU:CD1	2.75	0.49
2:D:328:GLU:O	2:D:329:SER:C	2.55	0.49
1:N:3:DT:H2"	1:N:4:DT:H5"	1.94	0.49
2:A:525:ASP:OD2	2:A:543:ARG:NH1	2.45	0.49
2:B:334:GLU:O	2:B:337:LEU:HB2	2.12	0.49
2:B:398:ILE:HD12	2:B:567:PHE:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:494:ASN:H	2:B:494:ASN:ND2	2.03	0.49
2:B:552:SER:O	2:B:553:GLY:C	2.55	0.49
2:C:427:ASN:ND2	2:C:517:PRO:HA	2.27	0.49
2:E:360:ASP:O	2:E:361:CYS:C	2.55	0.49
2:E:462:SER:O	2:E:464:PHE:N	2.46	0.49
2:K:328:GLU:O	2:K:329:SER:C	2.55	0.49
2:K:404:TYR:CD2	2:K:404:TYR:C	2.90	0.49
2:L:434:PRO:HD3	2:L:545:GLU:OE2	2.11	0.49
2:A:494:ASN:C	2:A:496:LEU:H	2.19	0.49
2:A:523:ASN:OD1	2:A:524:ILE:N	2.45	0.49
2:B:497:ASP:HB3	2:B:499:TYR:CD2	2.47	0.49
2:D:398:ILE:HD11	2:D:564:TRP:CD2	2.47	0.49
2:H:488:PHE:HB3	2:H:496:LEU:HD11	1.94	0.49
2:K:354:GLN:OE1	2:L:364:MET:HG2	2.13	0.49
2:B:529:GLU:CG	2:B:531:ARG:HE	2.25	0.49
2:D:548:CYS:O	2:D:550:ASP:N	2.45	0.49
2:G:377:SER:O	2:G:378:MET:C	2.55	0.49
2:G:378:MET:HB3	2:G:379:PRO:HD3	1.95	0.49
2:H:348:PHE:CD2	2:H:349:LEU:HD23	2.48	0.49
2:L:447:ILE:CG1	2:L:564:TRP:CE2	2.87	0.49
2:A:466:LEU:O	2:A:469:LEU:HB2	2.12	0.49
2:A:485:TRP:CD2	2:A:526:VAL:HG11	2.47	0.49
2:D:424:PRO:HB3	2:D:499:TYR:CE2	2.48	0.49
2:F:513:ILE:CG1	2:F:514:LYS:H	2.26	0.49
2:F:533:LEU:HA	2:F:536:HIS:CE1	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:L:476:LEU:HD13	2:L:476:LEU:C	2.38	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:I:316:MET:HE3	2:I:361:CYS:CB	2.43	0.49
2:I:459:ASN:C	2:I:461:LYS:H	2.21	0.49
1:M:3:DT:H2"	1:M:4:DT:H5"	1.95	0.49
2:G:441:MET:SD	2:G:441:MET:C	2.96	0.49
2:H:446:LEU:HB2	2:H:564:TRP:CZ2	2.48	0.49
2:I:427:ASN:HD21	2:I:517:PRO:CA	2.26	0.49
2:I:497:ASP:CG	2:I:538:ARG:HE	2.21	0.49
2:L:382:ILE:CG2	2:L:568:PHE:CD1	2.96	0.49
2:L:483:ALA:O	2:L:485:TRP:N	2.46	0.49
2:L:496:LEU:HD13	2:L:538:ARG:CD	2.41	0.49
2:L:534:TYR:C	2:L:536:HIS:H	2.21	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:545:GLU:N	2:L:546:GLN:OE1	2.46	0.49
2:B:316:MET:O	2:B:319:TRP:HB3	2.13	0.48
2:C:453:SER:CB	2:C:472:THR:HG21	2.37	0.48
2:C:559:ILE:HG23	2:C:563:ASP:HB2	1.94	0.48
2:E:552:SER:O	2:E:553:GLY:C	2.55	0.48
2:F:438:GLY:HA2	5:F:6:ADP:C4'	2.42	0.48
2:G:428:CYS:C	2:G:429:LEU:HD23	2.38	0.48
2:J:533:LEU:HA	2:J:536:HIS:CE1	2.49	0.48
2:L:567:PHE:HD2	2:L:568:PHE:HD2	1.60	0.48
2:F:541:THR:C	2:F:542:PHE:HD2	2.21	0.48
2:A:412:PHE:HA	2:A:542:PHE:CZ	2.48	0.48
2:A:446:LEU:HD13	2:A:564:TRP:CZ2	2.49	0.48
2:C:513:ILE:HG13	2:C:514:LYS:N	2.27	0.48
2:E:395:TRP:CE2	2:E:570:ARG:NE	2.80	0.48
2:L:488:PHE:C	2:L:538:ARG:HH22	2.22	0.48
2:B:378:MET:N	2:B:379:PRO:CD	2.76	0.48
2:F:401:PHE:HE2	2:F:544:PHE:CE2	2.32	0.48
2:F:412:PHE:HA	2:F:542:PHE:CE1	2.48	0.48
2:A:460:HIS:HA	2:A:465:TRP:CB	2.39	0.48
2:A:477:VAL:HG21	2:A:488:PHE:CZ	2.49	0.48
2:D:513:ILE:CD1	2:D:514:LYS:H	2.17	0.48
2:E:337:LEU:C	2:E:339:ALA:N	2.71	0.48
2:G:435:PRO:O	2:G:436:ASN:HB2	2.13	0.48
2:H:399:LEU:HD13	2:H:409:LEU:HD22	1.96	0.48
2:I:427:ASN:ND2	2:I:517:PRO:CA	2.74	0.48
2:J:311:PHE:CZ	2:J:313:PHE:HA	2.49	0.48
2:L:454:VAL:O	2:L:455:LEU:CG	2.55	0.48
2:A:347:ALA:O	2:A:350:ALA:HB3	2.13	0.48
2:A:460:HIS:ND1	2:A:460:HIS:N	2.62	0.48
2:C:382:ILE:HD11	2:C:420:LEU:HD22	1.96	0.48
2:F:418:LEU:HD22	2:F:426:LYS:HG2	1.96	0.48
2:F:457:PHE:CZ	2:F:484:CYS:HA	2.49	0.48
2:G:476:LEU:O	2:G:476:LEU:HD13	2.13	0.48
2:J:330:LYS:O	2:J:331:ILE:C	2.56	0.48
2:K:399:LEU:O	2:K:400:THR:C	2.55	0.48
2:K:485:TRP:CD2	2:K:526:VAL:HG11	2.47	0.48
2:L:410:ILE:O	2:L:410:ILE:HG12	2.12	0.48
2:L:458:ALA:O	2:L:459:ASN:C	2.56	0.48
2:B:442:LEU:O	2:B:443:CYS:C	2.55	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:421:LYS:HB2	2:D:423:ILE:HD12	1.95	0.48
2:E:309:GLU:O	2:E:310:LYS:C	2.56	0.48
2:G:453:SER:HB3	2:G:472:THR:CG2	2.43	0.48
2:G:489:ASP:O	2:G:493:ARG:NE	2.46	0.48
2:I:499:TYR:HB3	2:I:500:PRO:HD2	1.94	0.48
2:A:398:ILE:HG12	2:A:559:ILE:HD12	1.96	0.48
2:A:548:CYS:O	2:A:549:THR:C	2.57	0.48
2:C:337:LEU:C	2:C:339:ALA:H	2.22	0.48
2:F:377:SER:O	2:F:378:MET:C	2.55	0.48
2:F:435:PRO:HA	5:F:6:ADP:O3B	2.14	0.48
2:H:441:MET:HE2	2:H:441:MET:O	2.14	0.48
2:I:351:THR:HG21	2:I:357:HIS:CD2	2.48	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: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:D:477:VAL:HG21	2:D:488:PHE:HZ	1.79	0.48
2:E:362:ALA:O	2:E:363:THR:C	2.56	0.48
2:G:321:TYR:C	2:G:321:TYR:CD1	2.92	0.48
2:G:513:ILE:CG1	2:G:514:LYS:N	2.77	0.48
2:H:376:LEU:HB3	2:H:377:SER:H	1.42	0.48
2:H:401:PHE:CE2	2:H:544:PHE:CE2	3.02	0.48
2:H:460:HIS:C	2:H:462:SER:H	2.21	0.48
2:B:345:ALA:O	2:B:348:PHE:HB3	2.14	0.48
2:H:362:ALA:O	2:H:363:THR:C	2.57	0.48
2:H:566:SER:O	2:H:567:PHE:C	2.57	0.48
2:I:453:SER:CB	2:I:472:THR:HG21	2.42	0.48
2:L:383:LYS:HA	2:L:386:CYS:HB2	1.94	0.48
2:L:398:ILE:CG2	2:L:399:LEU:N	2.76	0.48
2:L:434:PRO:CB	2:L:437:THR:OG1	2.62	0.48
2:L:571:LEU:O	2:L:575:LEU:HB2	2.14	0.48
2:A:525:ASP:C	2:A:525:ASP:OD1	2.55	0.47
2:D:437:THR:OG1	2:D:439:LYS:HE2	2.14	0.47
2:D:553:GLY:O	2:D:554:GLU:C	2.57	0.47
2:H:351:THR:HG21	2:H:357:HIS:CD2	2.49	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:L:330:LYS:O	2:L:331:ILE:C	2.55	0.47
2:L:499:TYR:CB	2:L:500:PRO:CD	2.91	0.47
2:D:405:GLN:O	2:D:406:ASN:HB2	2.13	0.47
2:E:373:THR:HG23	2:E:381:TYR:CE1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:552:SER:O	2:I:554:GLU:N	2.39	0.47
2:K:318:GLN:O	2:K:319:TRP:C	2.57	0.47
2:K:395:TRP:CE2	2:K:570:ARG:NE	2.83	0.47
2:K:418:LEU:N	2:K:418:LEU:HD12	2.29	0.47
2:B:328:GLU:O	2:B:329:SER:C	2.57	0.47
2:B:351:THR:HG21	2:B:357:HIS:CD2	2.49	0.47
2:G:488:PHE:CE1	2:G:492:LEU:HD23	2.49	0.47
2:K:410:ILE:HG12	2:K:414:ASN:ND2	2.29	0.47
2:A:425:LYS:HE3	2:A:426:LYS:HE2	1.96	0.47
2:D:434:PRO:O	2:D:437:THR:HG23	2.13	0.47
2:E:419:TRP:CZ2	2:E:519:LEU:HG	2.49	0.47
2:F:419:TRP:CD1	2:F:429:LEU:HG	2.48	0.47
2:F:562:ALA:O	2:F:565:LYS:HB3	2.15	0.47
2:G:470:ALA:HA	2:G:513:ILE:HG21	1.96	0.47
2:J:368:TYR:O	2:J:372:GLU:HB2	2.14	0.47
2:D:366:ARG:O	2:D:367:HIS:C	2.56	0.47
2:E:419:TRP:CD1	2:E:429:LEU:HG	2.48	0.47
2:F:373:THR:C	2:F:375:ALA:N	2.71	0.47
2:F:377:SER:OG	2:F:379:PRO:HD2	2.14	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:J:432:ILE:HD12	2:J:541:THR:CG2	2.44	0.47
2:L:538:ARG:CG	2:L:539:VAL:HG23	2.42	0.47
2:C:332:ALA:HB2	2:C:358:VAL:CG1	2.43	0.47
2:C:432:ILE:HD12	2:C:541:THR:HG21	1.97	0.47
2:C:533:LEU:HA	2:C:536:HIS:CE1	2.50	0.47
2:E:328:GLU:O	2:E:329:SER:C	2.56	0.47
2:E:440:SER:N	5:E:5:ADP:O1B	2.44	0.47
2:F:319:TRP:HH2	2:F:334:GLU:HB3	1.80	0.47
2:G:395:TRP:NE1	2:G:570:ARG:HD3	2.30	0.47
2:G:432:ILE:HD12	2:G:541:THR:HG21	1.96	0.47
2:H:357:HIS:O	2:H:358:VAL:C	2.58	0.47
2:H:495:ALA:O	2:H:498:GLY:N	2.48	0.47
2:I:496:LEU:HD23	2:I:518:LEU:HD12	1.97	0.47
2:I:548:CYS:O	2:I:550:ASP:N	2.47	0.47
2:J:416:LEU:HD12	2:J:416:LEU:O	2.15	0.47
2:J:447:ILE:HG12	2:J:519:LEU:HD12	1.96	0.47
2:K:345:ALA:O	2:K:348:PHE:HB3	2.14	0.47
2:L:438:GLY:HA3	2:L:548:CYS:CB	2.45	0.47
2:L:465:TRP:CZ2	2:L:506:LYS:HB3	2.49	0.47
2:L:552:SER:O	2:L:553:GLY:C	2.57	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:503:ILE:CG1	2:A:513:ILE:HG22	2.45	0.47
2:A:565:LYS:O	2:A:569:VAL:HG23	2.15	0.47
2:B:327:GLU:O	2:B:328:GLU:C	2.56	0.47
2:F:366:ARG:O	2:F:367:HIS:C	2.57	0.47
2:G:362:ALA:O	2:G:363:THR:C	2.58	0.47
2:H:409:LEU:HG	2:H:413:ILE:HD11	1.97	0.47
2:H:427:ASN:CG	2:H:427:ASN:O	2.58	0.47
2:H:497:ASP:CG	2:H:538:ARG:HE	2.23	0.47
2:I:419:TRP:CD1	2:I:429:LEU:HG	2.50	0.47
2:J:335:TYR:CE2	2:J:345:ALA:HA	2.50	0.47
2:L:418:LEU:CD2	2:L:426:LYS:HD2	2.43	0.47
2:L:460:HIS:HE2	2:L:463:HIS:HB2	1.77	0.47
2:L:532:TYR:CB	2:L:535:LEU:HD13	2.44	0.47
1:N:7:DT:OP1	2:L:465:TRP:NE1	2.46	0.47
2:A:353:SER:O	2:A:357:HIS:CD2	2.68	0.47
2:A:439:LYS:HB2	5:A:1:ADP:O2B	2.15	0.47
2:C:316:MET:HE3	2:C:361:CYS:CB	2.45	0.47
2:D:399:LEU:O	2:D:401:PHE:N	2.48	0.47
2:D:541:THR:CG2	2:D:542:PHE:N	2.78	0.47
2:E:424:PRO:O	2:E:425:LYS:HB2	2.15	0.47
2:F:370:ARG:HG2	2:F:370:ARG:HH11	1.80	0.47
2:H:552:SER:O	2:H:553:GLY:C	2.58	0.47
2:I:377:SER:O	2:I:378:MET:C	2.57	0.47
2:I:505:ARG:CZ	2:I:511:VAL:HG23	2.44	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:A:370:ARG:HH11	2:F:329:SER:CB	2.28	0.47
2:A:442:LEU:O	2:A:443:CYS:C	2.58	0.47
2:A:555:GLN:HA	2:A:556:PRO:HD2	1.73	0.47
2:B:381:TYR:OH	2:B:450:LEU:O	2.28	0.47
2:C:453:SER:HA	2:D:512:GLN:HE22	1.80	0.47
2:D:398:ILE:HD12	2:D:567:PHE:HB2	1.97	0.47
2:E:425:LYS:HE2	2:E:538:ARG:CZ	2.45	0.47
2:F:337:LEU:C	2:F:339:ALA:N	2.73	0.47
2:F:490:THR:HG22	2:F:491:TYR:CD2	2.49	0.47
2:H:422:GLY:O	2:H:514:LYS:NZ	2.44	0.47
2:I:329:SER:HA	2:J:367:HIS:ND1	2.30	0.47
1:M:3:DT:H2''	1:M:4:DT:C5'	2.45	0.46
2:A:568:PHE:O	2:A:569:VAL:C	2.58	0.46
2:B:325:TYR:HE1	2:B:334:GLU:HG2	1.76	0.46
2:B:523:ASN:ND2	4:B:42:CL:CL	2.85	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:478:ASP:HB3	2:D:494:ASN:ND2	2.30	0.46
2:F:505:ARG:O	2:F:506:LYS:C	2.58	0.46
2:K:377:SER:CB	2:K:379:PRO:HD2	2.44	0.46
2:K:409:LEU:HG	2:K:413:ILE:HG13	1.97	0.46
2:L:416:LEU:CD1	2:L:419:TRP:CE3	2.99	0.46
2:B:316:MET:HE3	2:B:361:CYS:CB	2.42	0.46
2:B:453:SER:O	2:B:475:ALA:HA	2.15	0.46
2:I:463:HIS:C	2:I:465:TRP:H	2.24	0.46
2:J:361:CYS:O	2:J:365:VAL:HG23	2.15	0.46
2:L:458:ALA:C	2:L:460:HIS:N	2.72	0.46
2:A:481:THR:O	2:A:482:HIS:C	2.58	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:B:462:SER:C	2:B:464:PHE:H	2.22	0.46
2:I:418:LEU:HG	2:I:423:ILE:HD13	1.96	0.46
2:J:501:VAL:CG2	2:J:502:SER:N	2.78	0.46
2:A:447:ILE:HG12	2:A:519:LEU:HD12	1.97	0.46
2:E:373:THR:O	2:E:374:GLN:C	2.57	0.46
2:H:377:SER:O	2:H:378:MET:C	2.58	0.46
2:H:412:PHE:HA	2:H:542:PHE:CZ	2.50	0.46
2:K:379:PRO:O	2:K:380:ALA:C	2.59	0.46
2:B:317:VAL:O	2:B:318:GLN:C	2.56	0.46
2:D:325:TYR:HE1	2:D:334:GLU:HG2	1.77	0.46
2:H:425:LYS:HE2	2:H:537:SER:O	2.15	0.46
2:H:425:LYS:HE3	2:H:497:ASP:OD1	2.16	0.46
2:K:453:SER:OG	2:K:472:THR:HG21	2.15	0.46
2:L:380:ALA:HA	2:L:383:LYS:HG2	1.98	0.46
2:A:493:ARG:HD3	2:A:534:TYR:CE2	2.50	0.46
2:C:440:SER:O	2:C:441:MET:C	2.58	0.46
2:C:465:TRP:HZ2	2:C:487:TYR:CE2	2.33	0.46
2:I:331:ILE:HG22	2:I:332:ALA:N	2.30	0.46
2:I:377:SER:H	2:I:380:ALA:HB3	1.80	0.46
2:K:476:LEU:HD22	2:K:477:VAL: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:L:427:ASN:O	2:L:427:ASN:CG	2.57	0.46
2:L:476:LEU:HD22	2:L:477:VAL:N	2.27	0.46
2:B:543:ARG:O	2:B:544:PHE:HD1	1.99	0.46
2:H:418:LEU:N	2:H:418:LEU:CD1	2.78	0.46
2:I:354:GLN:O	2:I:355:ALA:C	2.58	0.46
2:J:437:THR:OG1	2:J:439:LYS:HE2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:570:ARG:C	2:L:572:TRP:H	2.24	0.46
2:B:337:LEU:C	2:B:339:ALA:H	2.23	0.46
2:L:380:ALA:O	2:L:383:LYS:N	2.49	0.46
2:L:442:LEU:HD13	2:L:557:PHE:O	2.16	0.46
2:L:494:ASN:C	2:L:496:LEU:N	2.74	0.46
2:B:499:TYR:HB3	2:B:500:PRO:CD	2.44	0.46
2:C:526:VAL:HG12	2:C:532:TYR:CD1	2.51	0.46
2:G:379:PRO:O	2:G:383:LYS:N	2.46	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:J:404:TYR:O	2:J:546:GLN:HG3	2.14	0.46
2:L:328:GLU:O	2:L:329:SER:C	2.59	0.46
2:L:420:LEU:C	2:L:422:GLY:N	2.72	0.46
2:A:427:ASN:CG	2:A:427:ASN:O	2.59	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
2:J:425:LYS:O	2:J:538:ARG:HA	2.16	0.46
2:L:382:ILE:HG21	2:L:568:PHE:CE1	2.51	0.46
2:L:525:ASP:C	2:L:525:ASP:OD1	2.59	0.46
2:B:330:LYS:O	2:B:331:ILE:C	2.59	0.45
2:B:361:CYS:O	2:B:365:VAL:HG23	2.15	0.45
2:E:505:ARG:NH1	2:E:511:VAL:HG23	2.31	0.45
2:F:348:PHE:CD2	2:F:349:LEU:HD23	2.51	0.45
2:G:497:ASP:OD1	2:G:538:ARG:HG2	2.16	0.45
2:H:307:GLN:C	2:H:308:THR:O	2.59	0.45
2:H:500:PRO:HA	2:H:514:LYS:HA	1.98	0.45
2:H:541:THR:C	2:H:542:PHE:HD2	2.24	0.45
2:I:315:THR:HB	2:I:344:ASN:ND2	2.31	0.45
2:I:419:TRP:CE2	2:I:517:PRO:HB3	2.51	0.45
2:J:572:TRP:CE2	2:J:577:LEU:HB3	2.51	0.45
2:L:499:TYR:CD1	2:L:500:PRO:HD2	2.52	0.45
2:L:573:GLY:C	2:L:575:LEU:H	2.23	0.45
2:A:441:MET:HE2	5:A:1:ADP:C8	2.51	0.45
2:G:571:LEU:CD2	2:G:574:ARG:HE	2.29	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:J:459:ASN:C	2:J:461:LYS:N	2.74	0.45
2:A:367:HIS:ND1	2:F:329:SER:HA	2.31	0.45
2:A:455:LEU:HB3	2:A:465:TRP:CE3	2.51	0.45
2:C:441:MET:C	2:C:441:MET:SD	3.00	0.45
2:D:440:SER:O	2:D:444:ASN:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:499:TYR:HB3	2:H:500:PRO:HD2	1.98	0.45
2:I:351:THR:HG21	2:I:357:HIS:NE2	2.31	0.45
2:J:453:SER:CB	2:J:472:THR:HG21	2.38	0.45
2:A:351:THR:HG21	2:A:357:HIS:CD2	2.51	0.45
2:B:409:LEU:O	2:B:410:ILE:C	2.60	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:337:LEU:C	2:L:339:ALA:N	2.74	0.45
2:A:372:GLU:O	2:A:376:LEU:CD2	2.65	0.45
2:B:501:VAL:HG11	2:B:515:ALA:HB2	1.98	0.45
5:C:3:ADP:H5'1	2:D:425:LYS:HD2	1.99	0.45
2:D:453:SER:CB	2:D:472:THR:HG21	2.46	0.45
2:E:332:ALA:HB2	2:E:358:VAL:HG11	1.99	0.45
2:G:459:ASN:O	2:G:465:TRP:HB3	2.17	0.45
2:H:442:LEU:O	2:H:445:SER:OG	2.32	0.45
2:K:361:CYS:O	2:K:365:VAL:HG23	2.16	0.45
2:L:387:LYS:O	2:L:387:LYS:HD2	2.16	0.45
2:L:417:LYS:HB3	2:L:418:LEU:HD12	1.97	0.45
2:L:559:ILE:CG2	2:L:560:THR:N	2.79	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
2:C:559:ILE:CG2	2:C:560:THR:N	2.77	0.45
2:D:378:MET:N	2:D:379:PRO:CD	2.79	0.45
2:F:562:ALA:O	2:F:565:LYS:N	2.50	0.45
2:J:447:ILE:HG13	2:J:476:LEU:CB	2.47	0.45
2:K:523:ASN:N	2:K:523:ASN:ND2	2.65	0.45
2:L:327:GLU:O	2:L:328:GLU:C	2.59	0.45
2:L:387:LYS:O	2:L:387:LYS:CD	2.64	0.45
1:N:5:DT:OP1	2:J:506:LYS:NZ	2.43	0.45
2:A:372:GLU:O	2:A:376:LEU:HD22	2.16	0.45
2:A:463:HIS:HB3	2:A:466:LEU:HD12	1.99	0.45
2:C:357:HIS:O	2:C:358:VAL:C	2.59	0.45
2:E:459:ASN:C	2:E:461:LYS:N	2.74	0.45
2:E:489:ASP:O	2:E:493:ARG:NE	2.47	0.45
2:F:432:ILE:HA	2:F:522:SER:O	2.16	0.45
2:G:337:LEU:C	2:G:339:ALA:H	2.25	0.45
2:K:457:PHE:CZ	2:K:484:CYS:HA	2.52	0.45
2:L:434:PRO:HG3	2:L:545:GLU:OE1	2.16	0.45
2:A:556:PRO:HB2	2:A:557:PHE:H	1.51	0.45
2:B:319:TRP:HH2	2:B:334:GLU:HB3	1.81	0.45
2:D:419:TRP:CZ2	2:D:519:LEU:HG	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:436:ASN:OD1	2:E:425:LYS:NZ	2.39	0.45
2:D:533:LEU:O	2:D:536:HIS:ND1	2.50	0.45
2:E:484:CYS:SG	2:E:488:PHE:HE2	2.40	0.45
2:F:418:LEU:H	2:F:418:LEU:CD1	2.29	0.45
2:L:466:LEU:CG	2:L:467:ALA:N	2.73	0.45
2:L:467:ALA:C	2:L:503:ILE:HG13	2.42	0.45
2:L:521:THR:O	2:L:522:SER:HB2	2.17	0.45
2:A:546:GLN:HA	2:A:547:PRO:HD3	1.75	0.45
2:G:319:TRP:HH2	2:G:334:GLU:HB3	1.82	0.45
2:H:519:LEU:HD23	2:H:519:LEU:HA	1.84	0.45
2:I:485:TRP:CD2	2:I:526:VAL:HG11	2.51	0.45
2:I:513:ILE:HD12	2:I:514:LYS:H	1.82	0.45
2:L:559:ILE:HG22	2:L:560:THR:N	2.31	0.45
2:A:321:TYR:C	2:A:321:TYR:CD1	2.95	0.45
2:A:441:MET:O	2:A:445:SER:N	2.23	0.45
2:B:313:PHE:O	2:B:314:GLY:C	2.60	0.45
2:B:440:SER:O	2:B:441:MET:C	2.61	0.45
2:D:462:SER:O	2:D:464:PHE:N	2.50	0.45
2:E:462:SER:C	2:E:464:PHE:N	2.73	0.45
2:F:441:MET:CB	5:F:6:ADP:H1'	2.47	0.45
2:J:568:PHE:O	2:J:569:VAL:C	2.60	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:L:383:LYS:O	2:L:386:CYS:N	2.50	0.45
2:L:405:GLN:OE1	2:L:546:GLN:OE1	2.35	0.45
2:A:523:ASN:OD1	2:A:524:ILE:HG13	2.17	0.44
2:C:373:THR:C	2:C:375:ALA:H	2.25	0.44
2:C:475:ALA:HB3	2:C:518:LEU:CD2	2.48	0.44
2:C:552:SER:O	2:C:553:GLY:C	2.59	0.44
2:D:395:TRP:CD2	2:D:570:ARG:HD2	2.52	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:G:466:LEU:HD22	2:G:469:LEU:CD1	2.47	0.44
5:H:8:ADP:O2A	2:I:425:LYS:HD2	2.18	0.44
2:J:564:TRP:O	2:J:567:PHE:HB3	2.17	0.44
2:K:434:PRO:O	2:K:437:THR:HG23	2.17	0.44
2:L:391:GLY:C	2:L:392:GLU:HG3	2.41	0.44
2:L:493:ARG:NH2	2:L:534:TYR:HD1	2.13	0.44
2:L:505:ARG:H	2:L:505:ARG:HG2	1.58	0.44
2:B:495:ALA:O	2:B:498:GLY:N	2.46	0.44
2:I:376:LEU:HD12	2:I:380:ALA:CB	2.39	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:378:MET:O	2:C:382:ILE:HG13	2.16	0.44
2:D:354:GLN:O	2:D:355:ALA:C	2.61	0.44
2:E:432:ILE:HD12	2:E:541:THR:CG2	2.47	0.44
2:J:449:PHE:CE2	2:J:568:PHE:CD2	3.06	0.44
2:K:485:TRP:CD2	2:K:526:VAL:CG1	3.00	0.44
2:A:378:MET:N	2:A:473:ARG:HH21	2.14	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:534:TYR:CZ	2:A:538:ARG:NH1	2.72	0.44
2:B:383:LYS:O	2:B:386:CYS:HB2	2.17	0.44
2:B:533:LEU:HA	2:B:536:HIS:CE1	2.53	0.44
2:E:395:TRP:CZ2	2:E:570:ARG:NE	2.86	0.44
2:F:476:LEU:HD22	2:F:477:VAL:C	2.42	0.44
2:I:505:ARG:CZ	2:I:511:VAL:CG2	2.95	0.44
2:J:335:TYR:C	2:J:337:LEU:N	2.75	0.44
2:L:354:GLN:O	2:L:355:ALA:C	2.60	0.44
2:D:418:LEU:HD12	2:D:418:LEU:N	2.33	0.44
2:E:441:MET:HE1	2:E:559:ILE:CB	2.47	0.44
2:E:464:PHE:C	2:E:466:LEU:H	2.26	0.44
2:G:465:TRP:NE1	2:G:466:LEU:HG	2.32	0.44
2:H:351:THR:HG21	2:H:357:HIS:NE2	2.32	0.44
2:I:465:TRP:O	2:I:465:TRP:CD2	2.70	0.44
2:J:464:PHE:HE1	2:J:505:ARG:O	2.01	0.44
2:K:379:PRO:O	2:K:382:ILE:N	2.50	0.44
2:L:466:LEU:C	2:L:468:SER:H	2.25	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:E:432:ILE:HA	2:E:522:SER:O	2.18	0.44
2:E:485:TRP:CD2	2:E:526:VAL:CG1	3.00	0.44
2:J:476:LEU:HD22	2:J:477:VAL:C	2.42	0.44
2:L:382:ILE:HG21	2:L:568:PHE:CD1	2.53	0.44
2:L:395:TRP:C	2:L:397:SER:N	2.75	0.44
2:L:437:THR:CG2	2:L:546:GLN:N	2.80	0.44
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:A:417:LYS:HG3	2:A:575:LEU:O	2.17	0.44
2:A:427:ASN:ND2	2:A:517:PRO:HA	2.32	0.44
2:D:377:SER:O	2:D:378:MET:C	2.60	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:482:HIS:CE1	2:D:524:ILE:HD13	2.53	0.44
2:F:493:ARG:O	2:F:496:LEU:HB2	2.18	0.44
2:J:351:THR:HG21	2:J:357:HIS:CD2	2.52	0.44
2:J:370:ARG:HG2	2:J:370:ARG:HH11	1.83	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:436:ASN:C	2:L:438:GLY:N	2.71	0.44
2:A:367:HIS:HE1	2:F:328:GLU:CB	2.30	0.44
2:A:567:PHE:O	2:A:571:LEU:HB2	2.18	0.44
2:F:525:ASP:OD2	2:F:543:ARG:NH1	2.51	0.44
2:J:432:ILE:O	2:J:543:ARG:HA	2.17	0.44
2:L:364:MET:O	2:L:367:HIS:HB2	2.18	0.44
2:L:405:GLN:NE2	2:L:544:PHE:HB3	2.33	0.44
2:A:358:VAL:O	2:A:359:LYS:C	2.59	0.44
2:A:476:LEU:HD23	2:A:519:LEU:HB3	1.99	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:B:441:MET:CE	2:B:559:ILE:H	2.31	0.44
2:B:560:THR:O	2:B:561:ASP:C	2.61	0.44
2:D:395:TRP:NE1	2:D:396:LYS:HG3	2.33	0.44
2:F:317:VAL:O	2:F:318:GLN:C	2.61	0.44
2:H:513:ILE:HD12	2:H:514:LYS:N	2.33	0.44
2:I:316:MET:O	2:I:317:VAL:C	2.61	0.44
2:I:464:PHE:CD2	2:I:506:LYS:CG	2.99	0.44
2:I:464:PHE:C	2:I:466:LEU:H	2.26	0.44
2:J:344:ASN:O	2:J:347:ALA:HB3	2.17	0.44
2:J:427:ASN:HD21	2:J:517:PRO:HA	1.82	0.44
2:L:315:THR:HB	2:L:344:ASN:ND2	2.32	0.44
1:M:4:DT:H2''	1:M:5:DT:O5'	2.18	0.43
2:D:532:TYR:HB3	2:D:535:LEU:HD12	2.00	0.43
2:E:457:PHE:CZ	2:E:484:CYS:HA	2.53	0.43
2:E:493:ARG:HD3	2:E:534:TYR:CE2	2.52	0.43
2:H:418:LEU:HG	2:H:423:ILE:HD12	1.99	0.43
2:K:316:MET:O	2:K:319:TRP:HB3	2.18	0.43
2:K:404:TYR:OH	2:K:547:PRO:O	2.26	0.43
2:B:565:LYS:O	2:B:566:SER:C	2.60	0.43
2:D:401:PHE:O	2:D:404:TYR:HB3	2.18	0.43
2:E:369:LEU:HA	2:E:369:LEU:HD23	1.75	0.43
2:H:490:THR:HG22	2:H:491:TYR:CD2	2.53	0.43
2:H:562:ALA:O	2:H:563:ASP:C	2.61	0.43
2:L:348:PHE:CZ	2:L:354:GLN:HB3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:459:ASN:O	2:A:465:TRP:HB3	2.18	0.43
2:B:443:CYS:O	2:B:444:ASN:C	2.62	0.43
2:B:447:ILE:HG13	2:B:476:LEU:CB	2.48	0.43
2:D:551:GLU:O	2:D:552:SER:CB	2.66	0.43
2:E:325:TYR:HE1	2:E:334:GLU:HG2	1.79	0.43
2:I:506:LYS:C	2:I:508:LYS:H	2.26	0.43
2:K:453:SER:H	2:K:472:THR:HG21	1.83	0.43
2:L:345:ALA:O	2:L:348:PHE:HB3	2.17	0.43
2:L:534:TYR:C	2:L:536:HIS:N	2.75	0.43
2:B:446:LEU:HB2	2:B:564:TRP:CZ2	2.53	0.43
2:B:458:ALA:HB2	2:C:491:TYR:HB3	2.01	0.43
2:C:559:ILE:HG23	2:C:563:ASP:CB	2.47	0.43
2:F:378:MET:O	2:F:382:ILE:HG13	2.18	0.43
2:F:557:PHE:HD2	2:F:558:ASN:H	1.67	0.43
2:I:377:SER:CB	2:I:379:PRO:HD2	2.48	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:L:370:ARG:HH21	2:L:471:ASP:CG	2.26	0.43
2:L:385:ARG:NH1	2:L:450:LEU:O	2.51	0.43
2:L:399:LEU:CD1	2:L:409:LEU:HD22	2.45	0.43
2:L:412:PHE:O	2:L:415:ALA:HB3	2.18	0.43
2:L:567:PHE:HD2	2:L:568:PHE:CD2	2.36	0.43
2:A:447:ILE:HG13	2:A:476:LEU:CB	2.48	0.43
2:B:432:ILE:HD12	2:B:541:THR:HG21	2.00	0.43
2:D:312:ASP:OD2	2:D:315:THR:OG1	2.29	0.43
2:D:349:LEU:HA	2:D:354:GLN:NE2	2.34	0.43
2:E:378:MET:N	2:E:379:PRO:CD	2.80	0.43
2:E:464:PHE:C	2:E:466:LEU:N	2.76	0.43
2:F:412:PHE:HA	2:F:542:PHE:CZ	2.54	0.43
2:F:441:MET:SD	2:F:441:MET:C	3.02	0.43
2:G:554:GLU:O	2:G:555:GLN:C	2.61	0.43
2:H:441:MET:CE	2:H:559:ILE:H	2.31	0.43
2:H:497:ASP:HB3	2:H:499:TYR:CD2	2.54	0.43
2:I:465:TRP:CG	2:I:465:TRP:O	2.71	0.43
2:I:558:ASN:CG	2:I:558:ASN:O	2.60	0.43
2:K:362:ALA:O	2:K:365:VAL:N	2.50	0.43
2:K:401:PHE:HE2	2:K:544:PHE:CE2	2.36	0.43
2:K:518:LEU:HD23	2:K:518:LEU:HA	1.86	0.43
2:L:568:PHE:O	2:L:572:TRP:HB2	2.17	0.43
2:A:328:GLU:CB	2:B:367:HIS:HE1	2.17	0.43
2:A:505:ARG:HG3	2:A:509:ALA:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:321:TYR:CD1	2:C:321:TYR:C	2.96	0.43
2:C:401:PHE:CE2	2:C:544:PHE:HE2	2.26	0.43
2:E:456:SER:OG	2:F:502:SER:HB3	2.18	0.43
2:G:475:ALA:HB3	2:G:518:LEU:CD2	2.48	0.43
2:I:459:ASN:C	2:I:461:LYS:N	2.76	0.43
2:K:525:ASP:OD1	2:K:527:GLN:HB2	2.19	0.43
2:L:434:PRO:CG	2:L:437:THR:HG21	2.48	0.43
2:L:552:SER:O	2:L:553:GLY:O	2.37	0.43
2:A:334:GLU:O	2:A:337:LEU:HB2	2.18	0.43
2:E:373:THR:C	2:E:375:ALA:N	2.76	0.43
2:F:429:LEU:HB2	2:F:519:LEU:HD23	2.00	0.43
2:G:328:GLU:O	2:G:329:SER:C	2.61	0.43
2:G:546:GLN:HA	2:G:547:PRO:HD3	1.77	0.43
2:H:459:ASN:OD1	2:I:463:HIS:HB2	2.18	0.43
2:I:500:PRO:HA	2:I:513:ILE:O	2.18	0.43
2:K:459:ASN:C	2:K:461:LYS:N	2.77	0.43
2:L:353:SER:O	2:L:357:HIS:CD2	2.71	0.43
2:L:448:HIS:CG	2:L:449:PHE:N	2.86	0.43
2:A:437:THR:HB	2:A:544:PHE:HB3	2.01	0.43
2:E:505:ARG:NH1	2:E:511:VAL:CG2	2.82	0.43
2:F:366:ARG:HG3	2:F:367:HIS:N	2.33	0.43
2:F:368:TYR:O	2:F:371:ALA:N	2.51	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:K:431:PHE:CE1	2:K:442:LEU:HD23	2.53	0.43
2:L:383:LYS:CG	2:L:384:ALA:N	2.82	0.43
2:L:503:ILE:HG22	2:L:511:VAL:HG12	2.01	0.43
2:B:477:VAL:O	2:B:520:VAL:HA	2.18	0.43
2:E:444:ASN:OD1	2:F:500:PRO:HD2	2.18	0.43
2:F:464:PHE:HE1	2:F:505:ARG:C	2.27	0.43
2:J:308:THR:C	2:J:310:LYS:H	2.27	0.43
2:K:439:LYS:HE3	5:L:11:ADP:O2B	2.18	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:499:TYR:CB	2:B:500:PRO:HD2	2.48	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:316:MET:O	2:I:319:TRP:HB3	2.19	0.43
2:I:541:THR:CG2	2:I:542:PHE:N	2.82	0.43
2:A:533:LEU:HD12	2:A:536:HIS:ND1	2.34	0.42
2:B:476:LEU:HD22	2:B:476:LEU:C	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:532:TYR:O	2:C:533:LEU:C	2.62	0.42
2:D:453:SER:H	2:D:472:THR:HG21	1.83	0.42
2:E:410:ILE:HG23	2:E:411:THR:N	2.33	0.42
2:E:543:ARG:H	2:E:543:ARG:HG2	1.72	0.42
2:G:399:LEU:O	2:G:400:THR:C	2.62	0.42
2:G:416:LEU:O	2:G:417:LYS:C	2.61	0.42
2:H:486:ARG:CZ	2:H:486:ARG:HB2	2.49	0.42
2:I:378:MET:N	2:I:379:PRO:CD	2.82	0.42
2:I:438:GLY:C	2:I:441:MET:HB3	2.44	0.42
2:K:439:LYS:HB2	5:L:11:ADP:O3B	2.19	0.42
2:K:486:ARG:NH1	2:K:486:ARG:HB2	2.33	0.42
2:B:464:PHE:CE2	2:B:506:LYS:HG2	2.54	0.42
2:D:377:SER:CB	2:D:379:PRO:HD2	2.49	0.42
2:F:457:PHE:O	2:F:460:HIS:HB3	2.19	0.42
2:G:493:ARG:O	2:G:497:ASP:OD2	2.37	0.42
2:H:328:GLU:HB3	2:I:367:HIS:CE1	2.54	0.42
2:H:457:PHE:C	2:H:459:ASN:N	2.76	0.42
2:I:377:SER:OG	2:I:379:PRO:HD2	2.18	0.42
2:I:489:ASP:O	2:I:493:ARG:NE	2.44	0.42
2:K:455:LEU:CD1	2:K:466:LEU:HD23	2.49	0.42
2:L:382:ILE:CG2	2:L:568:PHE:HD1	2.32	0.42
2:L:440:SER:HB2	2:L:444:ASN:H	1.84	0.42
2:L:534:TYR:CD2	2:L:534:TYR:O	2.73	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:D:566:SER:O	2:D:567:PHE:C	2.62	0.42
2:E:313:PHE:CE2	2:E:317:VAL:CG2	3.02	0.42
2:F:552:SER:C	2:F:554:GLU:H	2.27	0.42
2:G:555:GLN:C	2:G:557:PHE:H	2.27	0.42
2:H:454:VAL:HG23	2:I:512:GLN:OE1	2.19	0.42
2:I:370:ARG:HH21	2:I:511:VAL:HG11	1.83	0.42
2:I:395:TRP:CE2	2:I:570:ARG:NE	2.86	0.42
2:I:477:VAL:HG21	2:I:488:PHE:HZ	1.84	0.42
2:I:546:GLN:HA	2:I:547:PRO:HD3	1.85	0.42
2:J:464:PHE:HE1	2:J:505:ARG:C	2.27	0.42
2:J:485:TRP:CE3	2:J:526:VAL:HG11	2.54	0.42
2:B:401:PHE:CE2	2:B:544:PHE:CE2	3.05	0.42
2:C:371:ALA:C	2:C:373:THR:N	2.78	0.42
2:D:441:MET:CE	2:D:559:ILE:H	2.32	0.42
2:I:335:TYR:CE2	2:I:345:ALA:HA	2.54	0.42
2:I:395:TRP:H	2:I:566:SER:HB3	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:429:LEU:HB2	2:J:519:LEU:HD23	2.01	0.42
2:J:501:VAL:HG22	2:J:502:SER:N	2.34	0.42
2:K:453:SER:HB3	2:K:472:THR:HG21	2.00	0.42
2:L:440:SER:O	2:L:444:ASN:CG	2.63	0.42
2:A:441:MET:HG2	2:A:442:LEU:H	1.85	0.42
2:C:382:ILE:O	2:C:383:LYS:C	2.62	0.42
2:D:325:TYR:CZ	2:D:334:GLU:HG2	2.54	0.42
2:D:417:LYS:HG3	2:D:575:LEU:O	2.19	0.42
2:D:423:ILE:O	2:D:424:PRO:C	2.62	0.42
2:F:419:TRP:C	2:F:421:LYS:N	2.77	0.42
2:H:321:TYR:CD1	2:H:321:TYR:C	2.97	0.42
2:H:330:LYS:O	2:H:331:ILE:C	2.62	0.42
2:I:332:ALA:HB1	2:J:364:MET:HE1	2.01	0.42
1:N:1:DT:H72	1:N:2:DT:N3	2.28	0.42
2:A:503:ILE:HG13	2:A:513:ILE:CG2	2.50	0.42
2:F:313:PHE:O	2:F:315:THR:N	2.52	0.42
2:F:562:ALA:O	2:F:563:ASP:C	2.63	0.42
2:G:409:LEU:HD12	2:G:409:LEU:HA	1.86	0.42
2:G:475:ALA:HB3	2:G:518:LEU:HD23	2.01	0.42
2:I:335:TYR:O	2:I:338:ALA:N	2.53	0.42
2:J:370:ARG:HG3	2:J:471:ASP:OD2	2.19	0.42
2:J:447:ILE:HD13	2:J:447:ILE:HA	1.96	0.42
2:J:494:ASN:O	2:J:495:ALA:C	2.63	0.42
2:L:409:LEU:C	2:L:411:THR:H	2.28	0.42
2:L:574:ARG:CB	2:L:574:ARG:NH1	2.83	0.42
1:M:4:DT:H1'	1:M:5:DT:H5'	2.01	0.42
2:A:318:GLN:O	2:A:319:TRP:C	2.63	0.42
2:A:460:HIS:O	2:A:463:HIS:HA	2.20	0.42
2:B:362:ALA:O	2:B:363:THR:C	2.61	0.42
2:E:373:THR:HG23	2:E:381:TYR:HE1	1.84	0.42
2:E:376:LEU:O	2:E:473:ARG:NH2	2.53	0.42
2:F:454:VAL:HG13	2:F:476:LEU:HD13	2.02	0.42
2:F:533:LEU:HD12	2:F:536:HIS:ND1	2.35	0.42
2:H:492:LEU:N	2:H:492:LEU:CD1	2.82	0.42
2:I:566:SER:O	2:I:567:PHE:C	2.63	0.42
2:K:505:ARG:CZ	2:K:511:VAL:CG2	2.98	0.42
2:K:513:ILE:CG1	2:K:514:LYS:H	2.33	0.42
2:B:318:GLN:O	2:B:319:TRP:C	2.62	0.42
2:C:354:GLN:O	2:C:355:ALA:C	2.62	0.42
2:C:419:TRP:O	2:C:420:LEU:C	2.62	0.42
2:D:487:TYR:CE1	2:D:491:TYR:HD1	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:465:TRP:CE2	2:G:466:LEU:HG	2.54	0.42
2:G:555:GLN:C	2:G:557:PHE:N	2.78	0.42
2:I:321:TYR:CD1	2:I:321:TYR:C	2.97	0.42
2:K:455:LEU:HD21	2:K:475:ALA:CB	2.40	0.42
2:A:434:PRO:O	2:A:437:THR:HG23	2.20	0.42
2:B:378:MET:O	2:B:382:ILE:HG13	2.20	0.42
2:E:409:LEU:CD2	2:E:413:ILE:HD11	2.50	0.42
2:F:436:ASN:N	5:F:6:ADP:O2A	2.52	0.42
2:F:504:ASP:OD1	2:F:505:ARG:N	2.53	0.42
2:G:525:ASP:O	2:G:527:GLN:N	2.53	0.42
5:H:8:ADP:O2A	5:H:8:ADP:O3B	2.37	0.42
2:I:348:PHE:CZ	2:I:354:GLN:HB3	2.55	0.42
2:I:427:ASN:HD21	2:I:517:PRO:N	2.18	0.42
2:J:316:MET:HE3	2:J:361:CYS:CB	2.50	0.42
2:J:369:LEU:HA	2:J:369:LEU:HD23	1.79	0.42
2:J:418:LEU:HD12	2:J:418:LEU:N	2.35	0.42
2:K:401:PHE:CE2	2:K:544:PHE:CE2	3.08	0.42
2:K:418:LEU:HD12	2:K:418:LEU:H	1.85	0.42
2:K:459:ASN:O	2:K:460:HIS:C	2.62	0.42
2:K:482:HIS:CG	2:K:531:ARG:NH2	2.88	0.42
2:L:319:TRP:HH2	2:L:334:GLU:HB3	1.84	0.42
2:L:368:TYR:O	2:L:369:LEU:C	2.62	0.42
2:L:385:ARG:O	2:L:388:LEU:HB2	2.20	0.42
2:L:405:GLN:HA	2:L:546:GLN:NE2	2.35	0.42
2:L:424:PRO:O	2:L:425:LYS:HB2	2.20	0.42
2:A:434:PRO:O	2:A:435:PRO:C	2.63	0.42
2:A:568:PHE:O	2:A:572:TRP:N	2.52	0.42
2:C:398:ILE:HD12	2:C:567:PHE:HB2	2.02	0.42
2:C:476:LEU:C	2:C:476:LEU:CD2	2.92	0.42
2:D:506:LYS:O	2:D:508:LYS:N	2.50	0.42
2:E:571:LEU:O	2:E:572:TRP:C	2.63	0.42
2:F:311:PHE:CZ	2:F:313:PHE:HA	2.55	0.42
2:F:351:THR:HG22	2:F:353:SER:N	2.26	0.42
2:F:398:ILE:HD12	2:F:567:PHE:HB2	2.01	0.42
2:F:439:LYS:HB2	2:F:439:LYS:HE3	1.84	0.42
2:G:327:GLU:O	2:G:328:GLU:C	2.62	0.42
2:G:518:LEU:HD23	2:G:518:LEU:HA	1.85	0.42
2:H:378:MET:HG2	2:H:420:LEU:HB3	2.00	0.42
2:H:498:GLY:O	2:H:514:LYS:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:337:LEU:HD23	2:I:337:LEU:HA	1.92	0.42
2:I:454:VAL:HG22	2:I:476:LEU:HD12	2.02	0.42
2:I:478:ASP:HB3	2:J:494:ASN:HD21	1.85	0.42
2:K:492:LEU:O	2:K:495:ALA:HB3	2.19	0.42
2:L:452:GLY:H	2:L:474:ALA:HB3	1.85	0.42
2:A:351:THR:HG21	2:A:357:HIS:NE2	2.35	0.41
2:A:369:LEU:O	2:A:370:ARG:C	2.63	0.41
2:A:441:MET:CG	2:A:442:LEU:H	2.32	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:B:543:ARG:C	2:B:544:PHE:HD1	2.27	0.41
2:C:330:LYS:O	2:C:331:ILE:C	2.61	0.41
2:F:351:THR:HG21	2:F:357:HIS:CD2	2.55	0.41
2:F:453:SER:O	2:F:475:ALA:HA	2.20	0.41
2:K:366:ARG:O	2:K:367:HIS:C	2.62	0.41
2:K:482:HIS:CE1	2:K:524:ILE:HD13	2.55	0.41
2:L:438:GLY:C	2:L:440:SER:N	2.76	0.41
2:L:446:LEU:HD11	2:L:559:ILE:HB	1.93	0.41
2:A:519:LEU:HD23	2:A:519:LEU:HA	1.77	0.41
2:B:344:ASN:O	2:B:347:ALA:HB3	2.20	0.41
2:B:419:TRP:CD1	2:B:429:LEU:HG	2.56	0.41
2:C:500:PRO:HA	2:C:513:ILE:O	2.21	0.41
2:F:436:ASN:CA	5:F:6:ADP:O2A	2.66	0.41
2:G:495:ALA:O	2:G:498:GLY:N	2.41	0.41
2:K:413:ILE:HD13	2:K:571:LEU:HD22	2.02	0.41
2:K:464:PHE:O	2:K:466:LEU:N	2.53	0.41
1:M:3:DT:C4	1:M:4:DT:C4	3.08	0.41
2:A:473:ARG:O	2:A:517:PRO:HD2	2.19	0.41
2:C:372:GLU:O	2:C:376:LEU:HD13	2.20	0.41
2:D:370:ARG:O	2:D:371:ALA:C	2.62	0.41
2:G:490:THR:HG22	2:G:491:TYR:CE2	2.54	0.41
2:I:565:LYS:O	2:I:569:VAL:HG23	2.20	0.41
2:J:410:ILE:HG23	2:J:411:THR:N	2.36	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:K:460:HIS:O	2:K:461:LYS:C	2.64	0.41
2:B:321:TYR:CD1	2:B:321:TYR:C	2.97	0.41
2:B:501:VAL:CG1	2:B:515:ALA:HB2	2.50	0.41
2:F:361:CYS:O	2:F:365:VAL:HG23	2.20	0.41
2:F:450:LEU:HA	2:F:450:LEU:HD23	1.84	0.41
2:F:494:ASN:C	2:F:496:LEU:H	2.25	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:509:ALA:O	2:I:510:ALA:C	2.62	0.41
2:J:485:TRP:CD2	2:J:526:VAL:HG11	2.56	0.41
2:K:506:LYS:C	2:K:508:LYS:H	2.28	0.41
2:L:461:LYS:HZ3	2:L:483:ALA:HB1	1.85	0.41
2:B:351:THR:HG21	2:B:357:HIS:NE2	2.35	0.41
2:D:444:ASN:ND2	2:E:500:PRO:HD2	2.36	0.41
2:D:489:ASP:O	2:D:493:ARG:NE	2.51	0.41
2:E:313:PHE:O	2:E:314:GLY:C	2.63	0.41
2:E:331:ILE:HD13	2:E:361:CYS:SG	2.60	0.41
2:E:383:LYS:O	2:E:386:CYS:HB2	2.20	0.41
2:F:401:PHE:HZ	2:F:438:GLY:HA3	1.84	0.41
2:G:525:ASP:C	2:G:527:GLN:N	2.76	0.41
2:H:414:ASN:O	2:H:417:LYS:HB3	2.21	0.41
2:I:409:LEU:HG	2:I:413:ILE:HD11	2.03	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:K:509:ALA:O	2:K:510:ALA:C	2.64	0.41
2:L:465:TRP:CZ3	2:L:505:ARG:C	2.99	0.41
2:L:574:ARG:CZ	2:L:574:ARG:HB2	2.51	0.41
2:A:370:ARG:HD2	2:A:471:ASP:OD2	2.20	0.41
2:E:418:LEU:HD23	2:E:426:LYS:HD3	2.01	0.41
2:G:363:THR:HG22	2:G:367:HIS:CD2	2.55	0.41
2:G:446:LEU:HD23	2:G:519:LEU:HD11	2.02	0.41
2:G:485:TRP:CE3	2:G:526:VAL:HG11	2.56	0.41
2:G:506:LYS:O	2:G:507:HIS:HB2	2.20	0.41
2:G:525:ASP:O	2:G:526:VAL:C	2.63	0.41
2:H:435:PRO:O	2:H:436:ASN:HB2	2.19	0.41
2:H:447:ILE:HG13	2:H:476:LEU:CB	2.47	0.41
2:I:476:LEU:HD22	2:I:476:LEU:C	2.46	0.41
2:J:327:GLU:O	2:J:328:GLU:C	2.63	0.41
2:J:442:LEU:O	2:J:443:CYS:C	2.63	0.41
2:K:316:MET:O	2:K:317:VAL:C	2.62	0.41
2:K:319:TRP:HH2	2:K:334:GLU:HB3	1.86	0.41
2:K:476:LEU:O	2:K:476:LEU:HD13	2.20	0.41
2:L:467:ALA:O	2:L:469:LEU:N	2.52	0.41
2:A:353:SER:HB2	2:A:356:LYS:HB3	2.01	0.41
2:B:316:MET:O	2:B:317:VAL:C	2.64	0.41
2:B:482:HIS:CE1	2:B:531:ARG:NH2	2.89	0.41
2:E:331:ILE:O	2:E:332:ALA:C	2.64	0.41
2:E:363:THR:HG22	2:E:367:HIS:CD2	2.56	0.41
2:E:568:PHE:O	2:E:572:TRP:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:309:GLU:O	2:F:310:LYS:O	2.39	0.41
2:I:441:MET:HA	2:J:499:TYR:OH	2.21	0.41
2:J:378:MET:HB3	2:J:379:PRO:CD	2.45	0.41
2:J:423:ILE:HG23	2:J:424:PRO:HD2	2.02	0.41
2:J:446:LEU:HB2	2:J:564:TRP:CZ2	2.56	0.41
2:J:459:ASN:O	2:J:461:LYS:N	2.54	0.41
2:K:330:LYS:O	2:K:333:TYR:N	2.54	0.41
2:K:562:ALA:O	2:K:565:LYS:HB3	2.20	0.41
1:M:4:DT:C4'	2:E:507:HIS:CE1	3.00	0.41
2:B:418:LEU:CD1	2:B:418:LEU:H	2.32	0.41
2:C:337:LEU:C	2:C:339:ALA:N	2.78	0.41
2:E:339:ALA:HA	2:E:345:ALA:HB3	2.01	0.41
2:F:441:MET:HE3	2:F:558:ASN:HA	2.03	0.41
2:H:319:TRP:CH2	2:H:334:GLU:HB3	2.54	0.41
2:H:432:ILE:HG13	2:H:541:THR:HG23	2.03	0.41
2:K:424:PRO:C	2:K:426:LYS:H	2.28	0.41
2:K:543:ARG:HH11	2:K:543:ARG:CG	2.33	0.41
5:L:11:ADP:O1A	5:L:11:ADP:O1B	2.39	0.41
1:N:1:DT:C7	1:N:2:DT:N3	2.84	0.41
2:A:399:LEU:O	2:A:400:THR:C	2.63	0.41
2:A:461:LYS:HD2	2:A:461:LYS:HA	1.81	0.41
2:A:527:GLN:HA	2:A:536:HIS:HD2	1.86	0.41
2:B:335:TYR:C	2:B:337:LEU:N	2.78	0.41
2:B:418:LEU:HG	2:B:423:ILE:HD12	2.02	0.41
2:B:497:ASP:OD1	2:B:538:ARG:HG2	2.20	0.41
2:B:566:SER:O	2:B:567:PHE:C	2.64	0.41
2:C:439:LYS:CB	5:C:3:ADP:O2B	2.67	0.41
2:C:540:GLN:C	2:C:541:THR:OG1	2.64	0.41
2:D:335:TYR:O	2:D:336:ALA:C	2.64	0.41
2:D:337:LEU:HD23	2:D:337:LEU:HA	1.88	0.41
2:D:376:LEU:HD22	2:D:376:LEU:N	2.36	0.41
2:D:432:ILE:HA	2:D:522:SER:O	2.21	0.41
2:D:482:HIS:ND1	2:D:524:ILE:HD13	2.35	0.41
2:F:425:LYS:HE2	2:F:538:ARG:CZ	2.50	0.41
2:F:546:GLN:HA	2:F:547:PRO:HD3	1.92	0.41
2:G:492:LEU:N	2:G:492:LEU:CD1	2.83	0.41
2:G:543:ARG:HH11	2:G:543:ARG:HG2	1.86	0.41
2:H:378:MET:N	2:H:379:PRO:CD	2.84	0.41
2:H:398:ILE:HD12	2:H:567:PHE:HB2	2.02	0.41
2:H:457:PHE:CE1	2:H:460:HIS:CG	3.09	0.41
2:H:481:THR:HG21	2:I:490:THR:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:506:LYS:O	2:I:508:LYS:N	2.51	0.41
2:K:311:PHE:CE1	2:K:348:PHE:HB2	2.55	0.41
2:K:378:MET:N	2:K:379:PRO:HD3	2.36	0.41
2:L:332:ALA:HB2	2:L:358:VAL:HG11	2.02	0.41
2:L:375:ALA:C	2:L:376:LEU:HD22	2.46	0.41
2:L:395:TRP:O	2:L:396:LYS:C	2.64	0.41
2:L:437:THR:HG21	2:L:544:PHE:O	2.21	0.41
2:L:574:ARG:HH11	2:L:574:ARG:HB3	1.86	0.41
2:A:434:PRO:HD2	2:A:437:THR:HG21	2.03	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:D:562:ALA:O	2:D:565:LYS:HB3	2.21	0.41
2:E:398:ILE:HD12	2:E:567:PHE:HB2	2.02	0.41
2:E:410:ILE:HG12	2:E:414:ASN:ND2	2.36	0.41
2:E:513:ILE:HD12	2:E:513:ILE:HA	1.88	0.41
2:G:351:THR:HG21	2:G:357:HIS:CD2	2.56	0.41
2:G:466:LEU:HD22	2:G:469:LEU:HD11	2.03	0.41
2:G:566:SER:O	2:G:567:PHE:C	2.63	0.41
2:K:374:GLN:HE21	2:K:374:GLN:HB3	1.70	0.41
2:L:389:ALA:O	2:L:390:THR:C	2.62	0.41
2:L:395:TRP:N	2:L:566:SER:HB2	2.36	0.41
2:L:432:ILE:HD13	2:L:525:ASP:CA	2.46	0.41
5:A:1:ADP:N7	2:B:424:PRO:HG2	2.36	0.40
2:B:337:LEU:C	2:B:339:ALA:N	2.78	0.40
2:B:532:TYR:O	2:B:533:LEU:C	2.63	0.40
2:D:372:GLU:O	2:D:376:LEU:CD2	2.68	0.40
2:D:466:LEU:HB3	2:D:469:LEU:HD12	2.03	0.40
2:E:550:ASP:CB	2:E:556:PRO:HD3	2.51	0.40
2:F:531:ARG:NH1	2:K:404:TYR:HE1	2.18	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:H:409:LEU:HG	2:H:413:ILE:CD1	2.51	0.40
2:H:457:PHE:CE1	2:H:460:HIS:ND1	2.89	0.40
2:H:478:ASP:CB	2:I:494:ASN:HD21	2.34	0.40
2:H:492:LEU:O	2:H:493:ARG:C	2.64	0.40
2:I:335:TYR:C	2:I:337:LEU:N	2.79	0.40
2:J:425:LYS:HE2	2:J:538:ARG:NH1	2.37	0.40
2:J:556:PRO:HB2	2:J:557:PHE:CD1	2.56	0.40
2:J:562:ALA:O	2:J:563:ASP:C	2.64	0.40
2:K:364:MET:O	2:K:367:HIS:HB2	2.21	0.40
2:L:408:GLU:H	2:L:408:GLU:HG2	1.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:3:DT:H3'	2:I:464:PHE:CE2	2.51	0.40
2:B:434:PRO:O	2:B:435:PRO:C	2.61	0.40
2:B:485:TRP:O	2:B:486:ARG:C	2.64	0.40
2:C:378:MET:N	2:C:379:PRO:CD	2.84	0.40
2:D:462:SER:C	2:D:464:PHE:N	2.79	0.40
2:E:456:SER:HB2	2:F:502:SER:HB3	2.03	0.40
2:F:466:LEU:HA	2:F:466:LEU:HD23	1.83	0.40
2:G:501:VAL:HG22	2:G:502:SER:N	2.36	0.40
2:G:559:ILE:H	2:G:559:ILE:HG12	1.65	0.40
2:I:401:PHE:HE2	2:I:544:PHE:CE2	2.40	0.40
2:K:373:THR:O	2:K:374:GLN:C	2.64	0.40
2:K:485:TRP:O	2:K:486:ARG:C	2.61	0.40
2:L:317:VAL:O	2:L:318:GLN:C	2.64	0.40
2:L:448:HIS:C	2:L:450:LEU:H	2.29	0.40
2:B:509:ALA:O	2:B:510:ALA:C	2.64	0.40
2:D:462:SER:C	2:D:464:PHE:H	2.28	0.40
2:E:447:ILE:HG13	2:E:476:LEU:CB	2.51	0.40
2:E:547:PRO:C	2:E:549:THR:H	2.30	0.40
2:F:318:GLN:O	2:F:319:TRP:C	2.64	0.40
2:H:434:PRO:O	2:H:437:THR:HG23	2.20	0.40
2:J:316:MET:CE	2:J:361:CYS:HB2	2.50	0.40
2:J:490:THR:HG22	2:J:491:TYR:CD2	2.57	0.40
2:K:358:VAL:HG21	2:L:364:MET:HE1	2.02	0.40
2:K:419:TRP:O	2:K:420:LEU:C	2.64	0.40
2:L:450:LEU:HD23	2:L:450:LEU:HA	1.96	0.40
2:A:378:MET:HE1	2:A:473:ARG:HG3	2.03	0.40
2:C:317:VAL:O	2:C:318:GLN:C	2.63	0.40
2:C:354:GLN:OE1	2:D:364:MET:HG2	2.22	0.40
2:C:455:LEU:HD11	2:C:469:LEU:HD21	2.02	0.40
2:C:513:ILE:CG1	2:C:514:LYS:N	2.84	0.40
2:E:456:SER:C	2:E:458:ALA:N	2.79	0.40
2:F:418:LEU:CD2	2:F:426:LYS:HG2	2.52	0.40
2:I:485:TRP:CD2	2:I:526:VAL:CG1	3.05	0.40
2:I:534:TYR:O	2:I:538:ARG:NH1	2.54	0.40
2:K:331:ILE:HD13	2:K:361:CYS:SG	2.61	0.40
2:K:441:MET:HE1	2:K:559:ILE:H	1.87	0.40
2:K:459:ASN:OD1	2:L:464:PHE:CZ	2.74	0.40
2:L:394:SER:O	2:L:397:SER:HB2	2.20	0.40
2:L:499:TYR:CB	2:L:500:PRO:HD2	2.52	0.40
2:A:485:TRP:O	2:A:486:ARG:C	2.64	0.40
2:F:405:GLN:O	2:F:406:ASN:HB2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:412:PHE:HA	2:H:542:PHE:CE1	2.57	0.40
2:H:457:PHE:CE2	2:H:484:CYS:HA	2.56	0.40
2:J:345:ALA:O	2:J:348:PHE:HB3	2.22	0.40
2:J:505:ARG:NH1	2:J:511:VAL:HG23	2.36	0.40
2:K:506:LYS:O	2:K:508:LYS:N	2.55	0.40
2:L:405:GLN:HA	2:L:546:GLN:CD	2.46	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%)	3	19
2	B	268/274 (98%)	221 (82%)	40 (15%)	7 (3%)	4	21
2	C	268/274 (98%)	232 (87%)	32 (12%)	4 (2%)	8	33
2	D	268/274 (98%)	224 (84%)	31 (12%)	13 (5%)	1	11
2	E	272/274 (99%)	229 (84%)	34 (12%)	9 (3%)	3	17
2	F	268/274 (98%)	215 (80%)	40 (15%)	13 (5%)	1	11
2	G	268/274 (98%)	225 (84%)	37 (14%)	6 (2%)	5	25
2	H	272/274 (99%)	227 (84%)	38 (14%)	7 (3%)	4	21
2	I	268/274 (98%)	220 (82%)	39 (15%)	9 (3%)	3	16
2	J	268/274 (98%)	218 (81%)	42 (16%)	8 (3%)	3	19
2	K	271/274 (99%)	219 (81%)	42 (16%)	10 (4%)	2	15
2	L	268/274 (98%)	180 (67%)	60 (22%)	28 (10%)	0	2
All	All	3227/3288 (98%)	2622 (81%)	483 (15%)	122 (4%)	2	15

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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 ⓘ

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%)	207 (95%)	11 (5%)	22	50
2	B	218/230 (95%)	207 (95%)	11 (5%)	22	50
2	C	218/230 (95%)	206 (94%)	12 (6%)	19	47
2	D	218/230 (95%)	205 (94%)	13 (6%)	17	45
2	E	224/230 (97%)	206 (92%)	18 (8%)	11	35
2	F	218/230 (95%)	203 (93%)	15 (7%)	14	40
2	G	218/230 (95%)	206 (94%)	12 (6%)	19	47
2	H	224/230 (97%)	209 (93%)	15 (7%)	15	42
2	I	218/230 (95%)	208 (95%)	10 (5%)	24	53
2	J	218/230 (95%)	201 (92%)	17 (8%)	11	36
2	K	224/230 (97%)	207 (92%)	17 (8%)	12	37
2	L	218/230 (95%)	200 (92%)	18 (8%)	10	34
All	All	2634/2760 (95%)	2465 (94%)	169 (6%)	16	43

All (169) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	318	GLN
2	A	424	PRO
2	A	429	LEU
2	A	435	PRO
2	A	461	LYS
2	A	463	HIS
2	A	465	TRP
2	A	476	LEU
2	A	479	ASP
2	A	492	LEU
2	A	517	PRO
2	B	318	GLN
2	B	441	MET
2	B	473	ARG
2	B	476	LEU
2	B	479	ASP
2	B	492	LEU
2	B	494	ASN

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Mol	Chain	Res	Type
2	B	501	VAL
2	B	511	VAL
2	B	523	ASN
2	B	540	GLN
2	C	318	GLN
2	C	367	HIS
2	C	424	PRO
2	C	441	MET
2	C	473	ARG
2	C	476	LEU
2	C	479	ASP
2	C	492	LEU
2	C	502	SER
2	C	520	VAL
2	C	523	ASN
2	C	540	GLN
2	D	318	GLN
2	D	364	MET
2	D	424	PRO
2	D	441	MET
2	D	468	SER
2	D	471	ASP
2	D	473	ARG
2	D	476	LEU
2	D	479	ASP
2	D	492	LEU
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	473	ARG
2	E	476	LEU
2	E	479	ASP
2	E	492	LEU
2	E	501	VAL
2	E	505	ARG
2	E	506	LYS
2	E	513	ILE
2	E	520	VAL

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Mol	Chain	Res	Type
2	E	523	ASN
2	E	526	VAL
2	E	529	GLU
2	E	538	ARG
2	E	543	ARG
2	F	318	GLN
2	F	364	MET
2	F	376	LEU
2	F	441	MET
2	F	444	ASN
2	F	468	SER
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	G	318	GLN
2	G	364	MET
2	G	372	GLU
2	G	441	MET
2	G	468	SER
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	454	VAL
2	H	468	SER
2	H	473	ARG
2	H	476	LEU
2	H	479	ASP
2	H	492	LEU

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Mol	Chain	Res	Type
2	H	513	ILE
2	H	517	PRO
2	H	523	ASN
2	H	526	VAL
2	H	540	GLN
2	I	318	GLN
2	I	364	MET
2	I	441	MET
2	I	468	SER
2	I	473	ARG
2	I	476	LEU
2	I	479	ASP
2	I	523	ASN
2	I	526	VAL
2	I	540	GLN
2	J	318	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
2	J	479	ASP
2	J	492	LEU
2	J	501	VAL
2	J	505	ARG
2	J	513	ILE
2	J	523	ASN
2	J	526	VAL
2	J	538	ARG
2	J	543	ARG
2	J	548	CYS
2	K	306	LEU
2	K	318	GLN
2	K	441	MET
2	K	455	LEU
2	K	459	ASN
2	K	468	SER
2	K	473	ARG
2	K	476	LEU
2	K	479	ASP
2	K	492	LEU

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Mol	Chain	Res	Type
2	K	526	VAL
2	K	531	ARG
2	K	538	ARG
2	K	543	ARG
2	K	545	GLU
2	K	548	CYS
2	K	557	PHE
2	L	318	GLN
2	L	398	ILE
2	L	408	GLU
2	L	441	MET
2	L	449	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
2	L	575	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (85) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	403	ASN
2	A	427	ASN
2	A	482	HIS
2	A	512	GLN
2	B	318	GLN
2	B	367	HIS
2	B	403	ASN
2	B	436	ASN
2	B	494	ASN
2	B	523	ASN
2	B	536	HIS
2	B	546	GLN
2	B	558	ASN

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Mol	Chain	Res	Type
2	C	352	ASN
2	C	374	GLN
2	C	403	ASN
2	C	414	ASN
2	C	427	ASN
2	C	436	ASN
2	C	494	ASN
2	C	523	ASN
2	C	536	HIS
2	D	354	GLN
2	D	367	HIS
2	D	374	GLN
2	D	403	ASN
2	D	494	ASN
2	D	507	HIS
2	D	523	ASN
2	E	352	ASN
2	E	367	HIS
2	E	414	ASN
2	E	427	ASN
2	E	436	ASN
2	E	507	HIS
2	E	523	ASN
2	E	558	ASN
2	F	367	HIS
2	F	403	ASN
2	F	414	ASN
2	F	444	ASN
2	F	459	ASN
2	F	507	HIS
2	F	523	ASN
2	F	558	ASN
2	G	367	HIS
2	G	403	ASN
2	G	512	GLN
2	G	523	ASN
2	H	318	GLN
2	H	403	ASN
2	H	436	ASN
2	H	444	ASN
2	H	494	ASN
2	H	523	ASN

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Mol	Chain	Res	Type
2	H	536	HIS
2	H	558	ASN
2	I	357	HIS
2	I	374	GLN
2	I	403	ASN
2	I	427	ASN
2	I	444	ASN
2	I	494	ASN
2	I	523	ASN
2	I	536	HIS
2	J	403	ASN
2	J	427	ASN
2	J	494	ASN
2	J	507	HIS
2	J	523	ASN
2	J	546	GLN
2	K	367	HIS
2	K	374	GLN
2	K	403	ASN
2	K	414	ASN
2	K	427	ASN
2	K	523	ASN
2	L	367	HIS
2	L	414	ASN
2	L	459	ASN
2	L	460	HIS
2	L	463	HIS
2	L	523	ASN
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 oligosaccharides 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	H	8	3	28,29,29	1.06	3 (10%)	43,45,45	1.96	10 (23%)
5	ADP	E	5	3	28,29,29	1.07	2 (7%)	43,45,45	1.91	11 (25%)
5	ADP	G	7	3	28,29,29	1.16	4 (14%)	43,45,45	1.96	12 (27%)
5	ADP	C	3	3	28,29,29	1.04	4 (14%)	43,45,45	1.96	10 (23%)
5	ADP	J	9	3	28,29,29	1.08	3 (10%)	43,45,45	1.94	11 (25%)
5	ADP	D	4	3	28,29,29	1.09	2 (7%)	43,45,45	1.93	9 (20%)
5	ADP	L	11	3	28,29,29	1.98	8 (28%)	43,45,45	2.65	19 (44%)
5	ADP	K	10	3	28,29,29	1.14	2 (7%)	43,45,45	1.90	12 (27%)
5	ADP	A	1	3	28,29,29	1.04	1 (3%)	43,45,45	2.09	13 (30%)
5	ADP	F	6	-	28,29,29	1.12	2 (7%)	43,45,45	1.91	9 (20%)
5	ADP	B	2	3	28,29,29	1.02	3 (10%)	43,45,45	2.03	12 (27%)

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	H	8	3	-	1/16/32/32	0/3/3/3
5	ADP	E	5	3	-	1/16/32/32	0/3/3/3
5	ADP	G	7	3	-	1/16/32/32	0/3/3/3
5	ADP	C	3	3	-	1/16/32/32	0/3/3/3
5	ADP	J	9	3	-	1/16/32/32	0/3/3/3
5	ADP	D	4	3	-	0/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	ADP	L	11	3	-	4/16/32/32	0/3/3/3
5	ADP	K	10	3	-	1/16/32/32	0/3/3/3
5	ADP	A	1	3	-	1/16/32/32	0/3/3/3
5	ADP	F	6	-	-	0/16/32/32	0/3/3/3
5	ADP	B	2	3	-	1/16/32/32	0/3/3/3

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	11	ADP	PA-O3A	-6.46	1.52	1.59
5	L	11	ADP	O4'-C1'	3.23	1.49	1.42
5	F	6	ADP	PA-O3A	2.93	1.62	1.59
5	K	10	ADP	PA-O3A	2.84	1.62	1.59
5	G	7	ADP	C5-N7	-2.83	1.33	1.39
5	L	11	ADP	C5'-C4'	-2.82	1.43	1.51
5	L	11	ADP	PB-O3B	2.76	1.65	1.54
5	J	9	ADP	PA-O3A	2.56	1.62	1.59
5	G	7	ADP	O4'-C1'	2.54	1.47	1.42
5	L	11	ADP	C2'-C3'	2.52	1.60	1.53
5	E	5	ADP	PA-O3A	2.45	1.62	1.59
5	L	11	ADP	C2'-C1'	2.42	1.61	1.53
5	D	4	ADP	PA-O3A	2.38	1.62	1.59
5	L	11	ADP	C6-N6	2.37	1.40	1.34
5	A	1	ADP	O4'-C1'	2.34	1.47	1.42
5	F	6	ADP	C5-C4	2.29	1.43	1.39
5	B	2	ADP	O4'-C1'	2.28	1.47	1.42
5	C	3	ADP	O4'-C1'	2.27	1.47	1.42
5	J	9	ADP	O4'-C1'	2.26	1.47	1.42
5	L	11	ADP	C5-C6	2.26	1.47	1.41
5	B	2	ADP	C5-N7	-2.22	1.35	1.39
5	C	3	ADP	C6-N6	2.20	1.39	1.34
5	G	7	ADP	PA-O3A	2.20	1.61	1.59
5	H	8	ADP	PA-O3A	-2.16	1.57	1.59
5	C	3	ADP	PB-O3B	2.11	1.62	1.54
5	D	4	ADP	O4'-C1'	2.10	1.46	1.42
5	K	10	ADP	C6-N6	2.09	1.39	1.34
5	G	7	ADP	C6-N6	2.09	1.39	1.34
5	B	2	ADP	PB-O3B	2.09	1.62	1.54
5	E	5	ADP	O4'-C1'	2.08	1.46	1.42
5	C	3	ADP	C5-C4	2.03	1.42	1.39
5	H	8	ADP	C6-N6	2.01	1.39	1.34
5	J	9	ADP	C5-N7	-2.01	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	8	ADP	C5-C4	2.00	1.42	1.39

All (128) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	11	ADP	C5-C4-N3	-6.09	118.34	126.72
5	H	8	ADP	C5-C4-N3	-5.34	119.36	126.72
5	D	4	ADP	C5-C4-N3	-5.33	119.38	126.72
5	C	3	ADP	C5-C4-N3	-5.26	119.47	126.72
5	B	2	ADP	C5-C4-N3	-5.26	119.48	126.72
5	F	6	ADP	C5-C4-N3	-5.15	119.62	126.72
5	J	9	ADP	C5-C4-N3	-5.15	119.63	126.72
5	G	7	ADP	N3-C2-N1	-5.06	120.92	128.58
5	E	5	ADP	C5-C4-N3	-5.04	119.77	126.72
5	A	1	ADP	C5-C4-N3	-5.03	119.80	126.72
5	L	11	ADP	N3-C4-N9	5.01	135.69	127.17
5	E	5	ADP	N3-C2-N1	-4.94	121.10	128.58
5	L	11	ADP	C4'-O4'-C1'	-4.94	98.57	109.47
5	B	2	ADP	N3-C2-N1	-4.91	121.16	128.58
5	J	9	ADP	N3-C2-N1	-4.87	121.21	128.58
5	G	7	ADP	C5-C4-N3	-4.86	120.02	126.72
5	F	6	ADP	N3-C2-N1	-4.80	121.32	128.58
5	A	1	ADP	N3-C2-N1	-4.79	121.33	128.58
5	H	8	ADP	N3-C2-N1	-4.79	121.33	128.58
5	D	4	ADP	N3-C2-N1	-4.76	121.38	128.58
5	C	3	ADP	N3-C2-N1	-4.72	121.44	128.58
5	K	10	ADP	C5-C4-N3	-4.71	120.23	126.72
5	H	8	ADP	N3-C4-N9	4.68	135.13	127.17
5	K	10	ADP	N3-C2-N1	-4.66	121.53	128.58
5	L	11	ADP	N3-C2-N1	-4.59	121.63	128.58
5	D	4	ADP	N3-C4-N9	4.59	134.97	127.17
5	L	11	ADP	C2-N3-C4	4.52	122.87	111.83
5	J	9	ADP	N3-C4-N9	4.47	134.77	127.17
5	B	2	ADP	N3-C4-N9	4.46	134.76	127.17
5	C	3	ADP	N3-C4-N9	4.44	134.72	127.17
5	E	5	ADP	N3-C4-N9	4.29	134.47	127.17
5	L	11	ADP	C5-N7-C8	4.19	110.03	103.45
5	F	6	ADP	N3-C4-N9	4.17	134.26	127.17
5	A	1	ADP	N3-C4-N9	4.12	134.17	127.17
5	L	11	ADP	O2A-PA-O3A	-4.09	96.21	107.27
5	G	7	ADP	N3-C4-N9	4.08	134.10	127.17
5	B	2	ADP	C5-N7-C8	4.01	109.75	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	6	ADP	C2-N3-C4	3.97	121.52	111.83
5	C	3	ADP	C2-N3-C4	3.90	121.36	111.83
5	K	10	ADP	N3-C4-N9	3.87	133.76	127.17
5	H	8	ADP	C2-N3-C4	3.87	121.28	111.83
5	B	2	ADP	C2-N3-C4	3.85	121.25	111.83
5	A	1	ADP	C2-N3-C4	3.85	121.23	111.83
5	D	4	ADP	C2-N3-C4	3.83	121.19	111.83
5	J	9	ADP	C2-N3-C4	3.80	121.11	111.83
5	E	5	ADP	C2-N3-C4	3.78	121.06	111.83
5	K	10	ADP	C5-N7-C8	3.73	109.31	103.45
5	C	3	ADP	C5-N7-C8	3.73	109.31	103.45
5	H	8	ADP	C5-N7-C8	3.72	109.30	103.45
5	J	9	ADP	C5-N7-C8	3.71	109.28	103.45
5	G	7	ADP	C2-N3-C4	3.68	120.82	111.83
5	D	4	ADP	C5-N7-C8	3.67	109.22	103.45
5	L	11	ADP	N9-C8-N7	-3.66	108.74	113.94
5	L	11	ADP	O2'-C2'-C1'	3.64	122.65	110.10
5	F	6	ADP	C5-N7-C8	3.63	109.15	103.45
5	G	7	ADP	C5-N7-C8	3.59	109.09	103.45
5	K	10	ADP	C2-N3-C4	3.59	120.60	111.83
5	A	1	ADP	C2'-C1'-N9	-3.56	104.45	113.30
5	L	11	ADP	PA-O5'-C5'	-3.54	101.07	121.35
5	A	1	ADP	C5-N7-C8	3.49	108.93	103.45
5	E	5	ADP	C5-N7-C8	3.48	108.92	103.45
5	L	11	ADP	O3'-C3'-C4'	3.45	120.99	111.08
5	A	1	ADP	PA-O5'-C5'	-3.30	102.45	121.35
5	L	11	ADP	C4-C5-N7	-3.17	106.96	110.58
5	K	10	ADP	C4-C5-N7	-3.13	107.00	110.58
5	A	1	ADP	O4'-C1'-N9	3.12	114.09	108.09
5	H	8	ADP	PA-O5'-C5'	-3.01	104.13	121.35
5	F	6	ADP	C4-C5-N7	-2.99	107.16	110.58
5	C	3	ADP	C4-C5-N7	-2.98	107.17	110.58
5	B	2	ADP	C2'-C1'-N9	-2.94	105.99	113.30
5	G	7	ADP	C2'-C3'-C4'	2.93	108.27	102.61
5	L	11	ADP	C4-N9-C1'	-2.90	119.85	126.63
5	B	2	ADP	C4-C5-N7	-2.89	107.28	110.58
5	D	4	ADP	C4-C5-N7	-2.85	107.32	110.58
5	A	1	ADP	C2'-C3'-C4'	2.82	108.06	102.61
5	L	11	ADP	O4'-C4'-C5'	2.82	118.36	109.33
5	J	9	ADP	C4-C5-N7	-2.82	107.36	110.58
5	H	8	ADP	C4-C5-N7	-2.79	107.40	110.58
5	B	2	ADP	N9-C8-N7	-2.78	109.99	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1	ADP	C4-C5-N7	-2.74	107.45	110.58
5	G	7	ADP	PA-O5'-C5'	-2.74	105.66	121.35
5	D	4	ADP	PA-O5'-C5'	-2.73	105.69	121.35
5	C	3	ADP	PA-O5'-C5'	-2.72	105.74	121.35
5	B	2	ADP	C2'-C3'-C4'	2.72	107.87	102.61
5	F	6	ADP	PA-O5'-C5'	-2.71	105.82	121.35
5	A	1	ADP	N9-C8-N7	-2.68	110.13	113.94
5	L	11	ADP	O5'-C5'-C4'	2.66	118.05	108.99
5	L	11	ADP	O2A-PA-O5'	-2.65	95.56	107.57
5	E	5	ADP	C4-C5-N7	-2.64	107.56	110.58
5	J	9	ADP	C3'-C2'-C1'	2.64	106.45	101.46
5	G	7	ADP	O4'-C1'-N9	2.60	113.09	108.09
5	G	7	ADP	C4-C5-N7	-2.59	107.62	110.58
5	E	5	ADP	C2'-C1'-N9	-2.59	106.86	113.30
5	K	10	ADP	N9-C8-N7	-2.58	110.27	113.94
5	D	4	ADP	C3'-C2'-C1'	2.57	106.32	101.46
5	E	5	ADP	N9-C8-N7	-2.57	110.30	113.94
5	C	3	ADP	N9-C8-N7	-2.53	110.35	113.94
5	E	5	ADP	C3'-C2'-C1'	2.50	106.18	101.46
5	F	6	ADP	N9-C8-N7	-2.49	110.41	113.94
5	B	2	ADP	PA-O5'-C5'	-2.49	107.10	121.35
5	H	8	ADP	C3'-C2'-C1'	2.47	106.13	101.46
5	G	7	ADP	C2'-C1'-N9	-2.46	107.20	113.30
5	J	9	ADP	C2'-C1'-N9	-2.45	107.22	113.30
5	L	11	ADP	C4-N9-C8	2.44	108.30	105.74
5	G	7	ADP	N9-C8-N7	-2.44	110.48	113.94
5	J	9	ADP	N9-C8-N7	-2.40	110.54	113.94
5	K	10	ADP	C3'-C2'-C1'	2.37	105.95	101.46
5	F	6	ADP	C3'-C2'-C1'	2.36	105.93	101.46
5	L	11	ADP	C2'-C1'-N9	2.35	119.13	113.30
5	K	10	ADP	C2'-C1'-N9	-2.34	107.50	113.30
5	C	3	ADP	C2'-C3'-C4'	2.34	107.12	102.61
5	H	8	ADP	N9-C8-N7	-2.33	110.62	113.94
5	K	10	ADP	PA-O5'-C5'	-2.33	108.02	121.35
5	B	2	ADP	O4'-C1'-N9	2.32	112.55	108.09
5	J	9	ADP	PA-O5'-C5'	-2.30	108.14	121.35
5	E	5	ADP	C2'-C3'-C4'	2.29	107.03	102.61
5	K	10	ADP	C2'-C3'-C4'	2.26	106.98	102.61
5	D	4	ADP	N9-C8-N7	-2.25	110.75	113.94
5	H	8	ADP	C2'-C1'-N9	-2.24	107.74	113.30
5	B	2	ADP	C3'-C2'-C1'	2.23	105.69	101.46
5	J	9	ADP	C2'-C3'-C4'	2.19	106.84	102.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	11	ADP	C1'-N9-C8	2.14	131.85	127.09
5	A	1	ADP	C3'-C2'-C1'	2.12	105.48	101.46
5	E	5	ADP	PA-O5'-C5'	-2.12	109.22	121.35
5	C	3	ADP	C3'-C2'-C1'	2.11	105.46	101.46
5	G	7	ADP	O3B-PB-O3A	2.10	111.69	104.64
5	A	1	ADP	O3B-PB-O3A	2.05	111.50	104.64
5	K	10	ADP	O4'-C1'-N9	2.03	111.98	108.09

There are no chirality outliers.

All (12) torsion outliers are listed below:

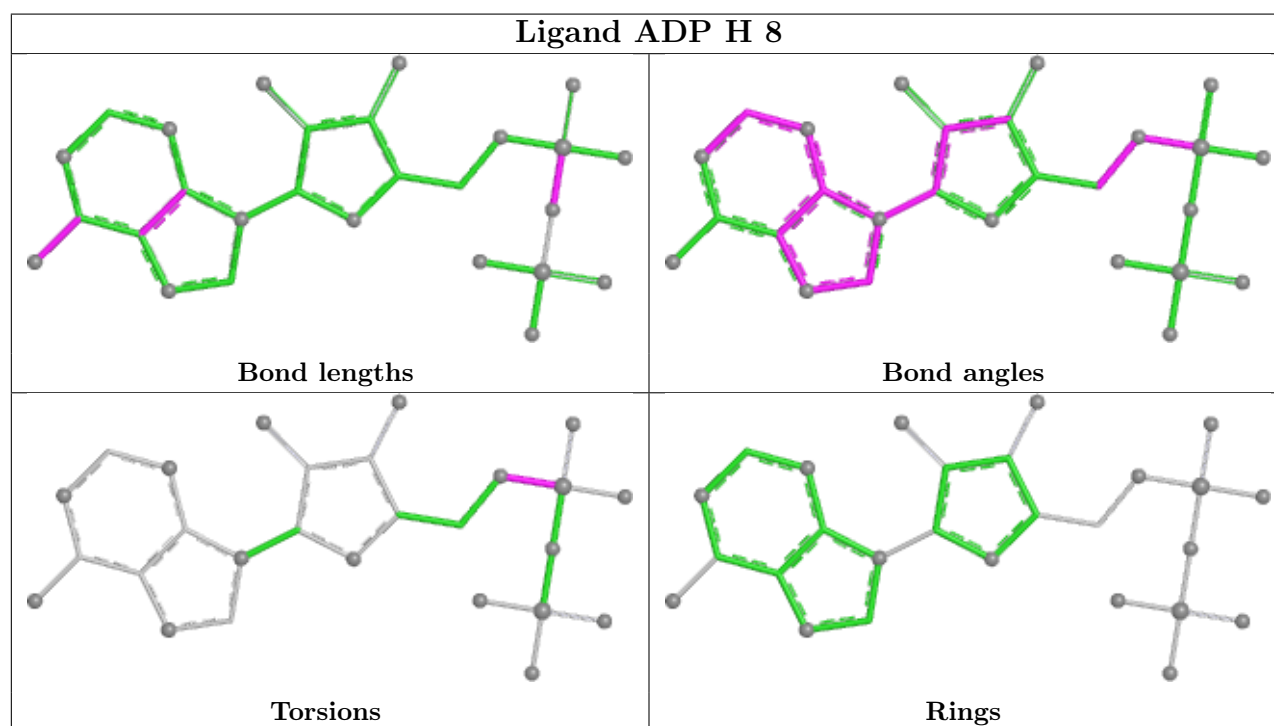
Mol	Chain	Res	Type	Atoms
5	A	1	ADP	C5'-O5'-PA-O1A
5	B	2	ADP	C5'-O5'-PA-O1A
5	C	3	ADP	C5'-O5'-PA-O1A
5	G	7	ADP	C5'-O5'-PA-O1A
5	L	11	ADP	C5'-O5'-PA-O1A
5	L	11	ADP	C5'-O5'-PA-O2A
5	L	11	ADP	C2'-C1'-N9-C8
5	L	11	ADP	C2'-C1'-N9-C4
5	E	5	ADP	C5'-O5'-PA-O1A
5	H	8	ADP	C5'-O5'-PA-O1A
5	J	9	ADP	C5'-O5'-PA-O1A
5	K	10	ADP	C5'-O5'-PA-O1A

There are no ring outliers.

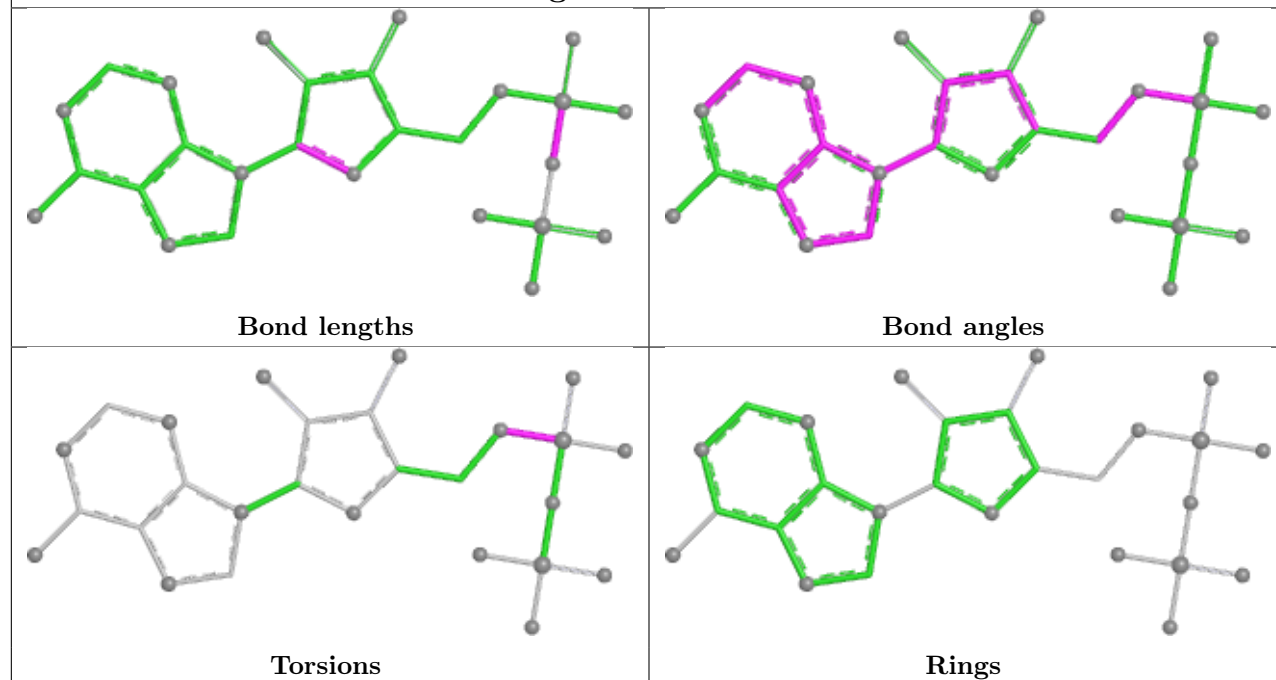
11 monomers are involved in 42 short contacts:

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

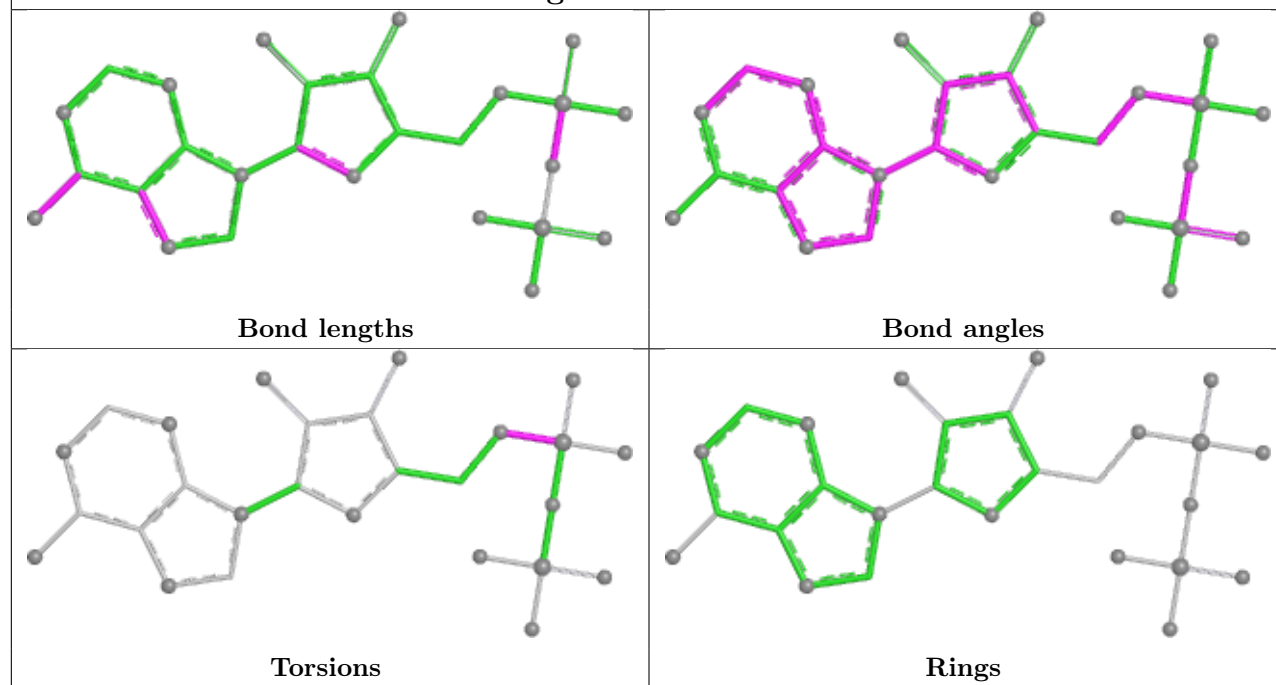
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



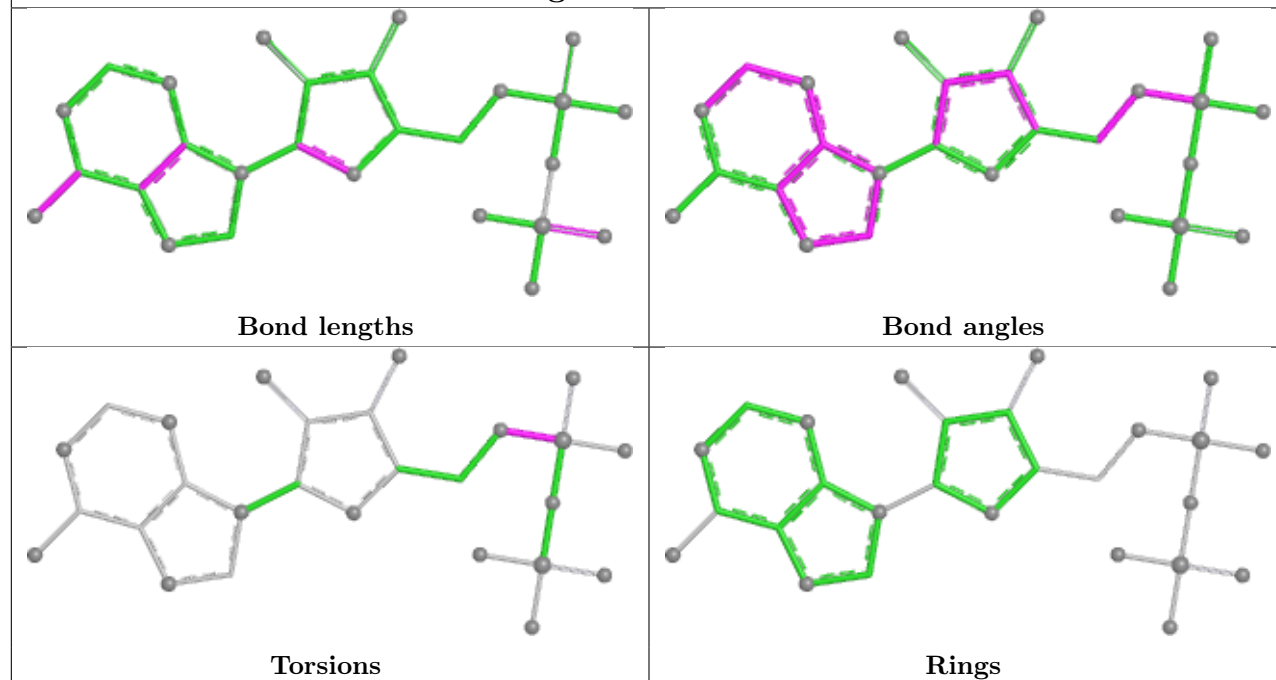
Ligand ADP E 5



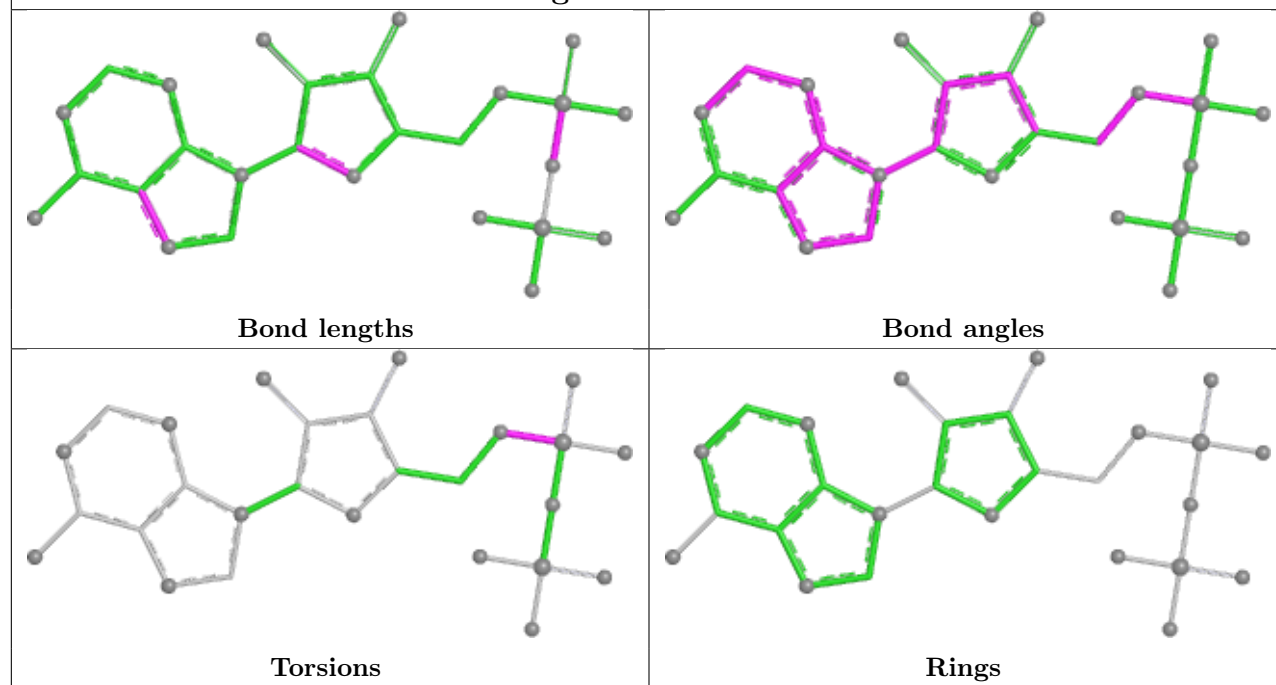
Ligand ADP G 7



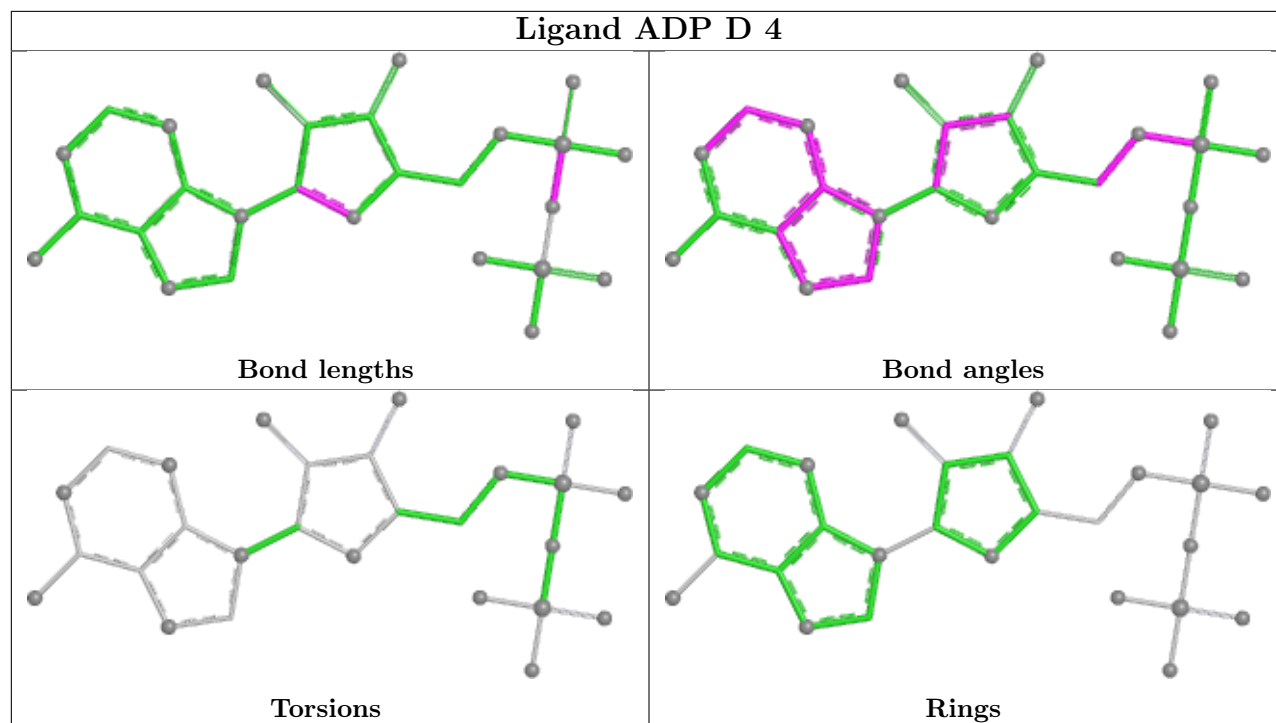
Ligand ADP C 3



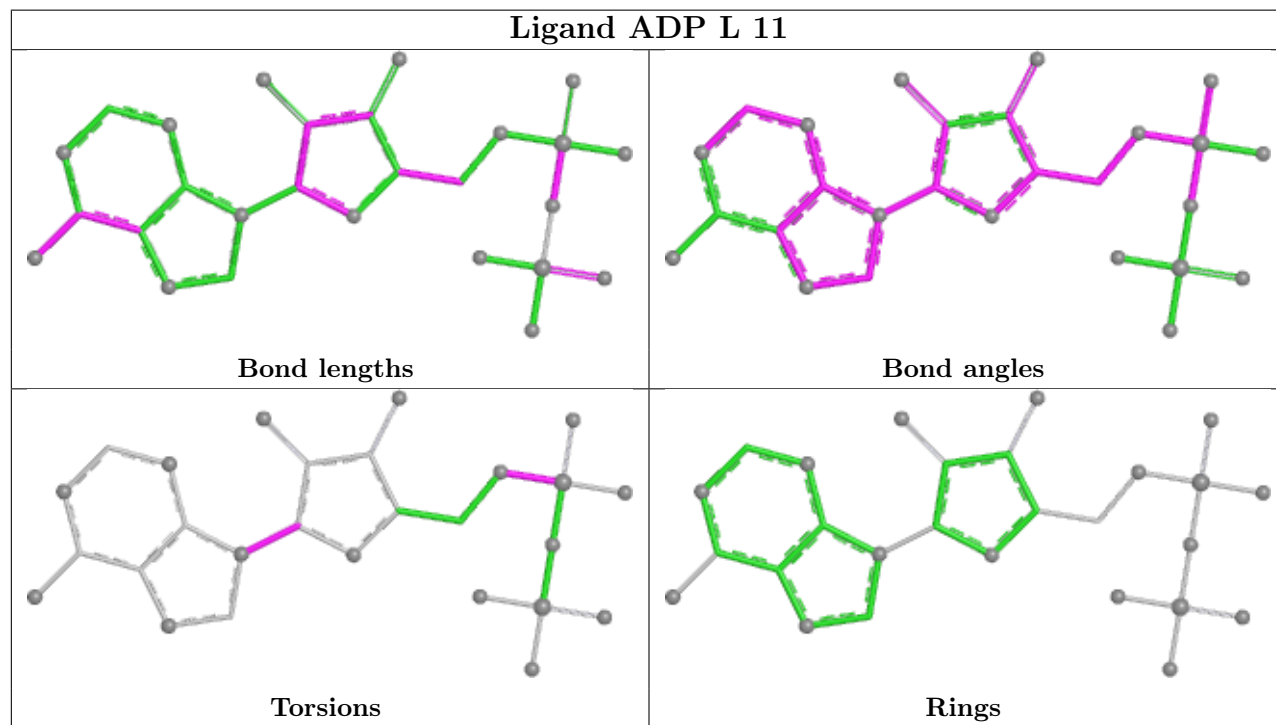
Ligand ADP J 9



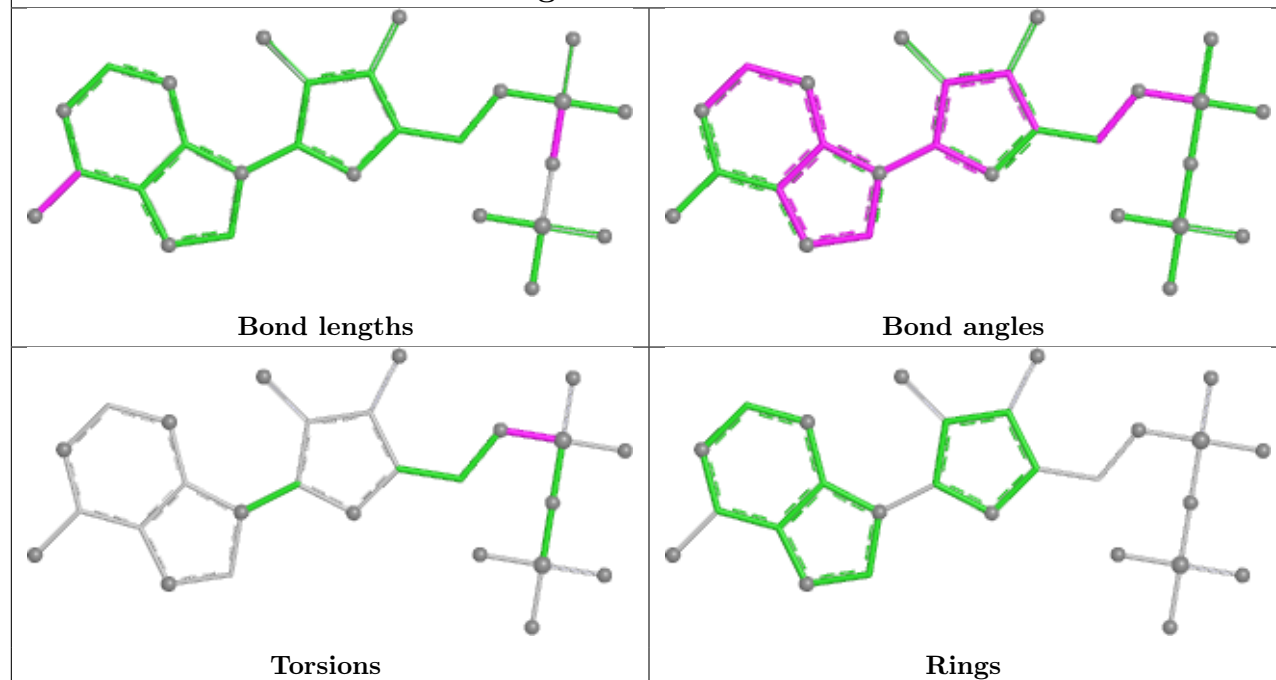
Ligand ADP D 4



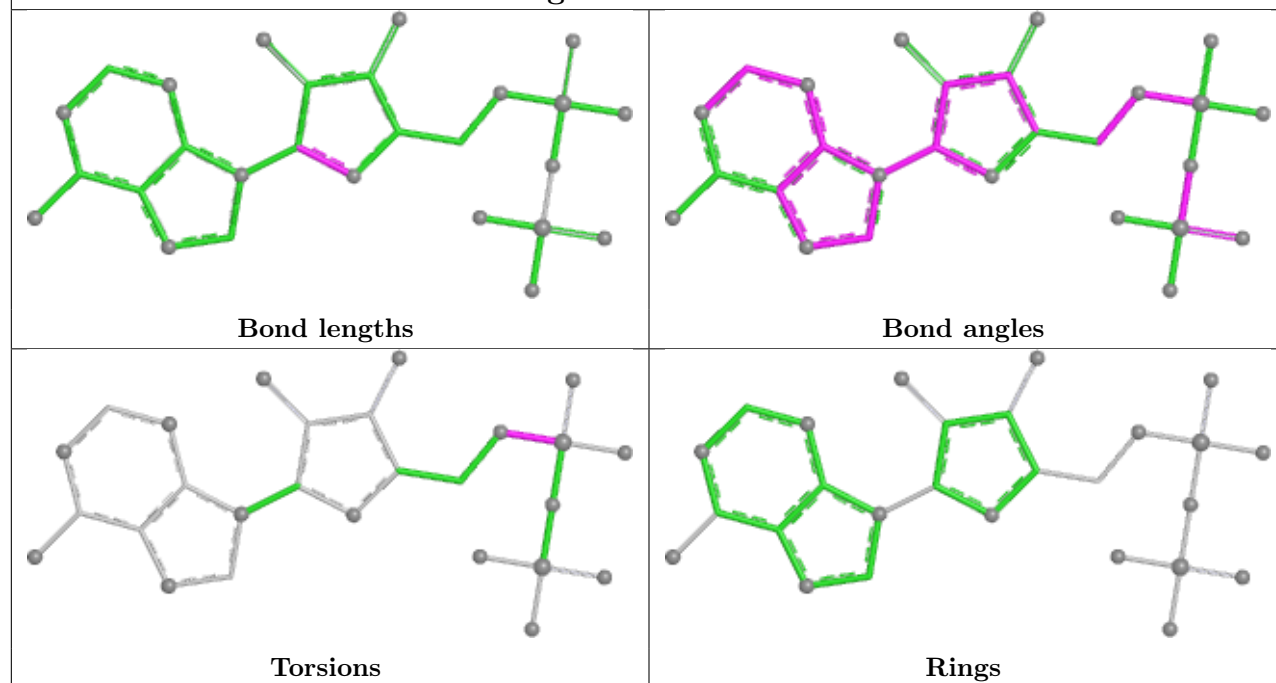
Ligand ADP L 11

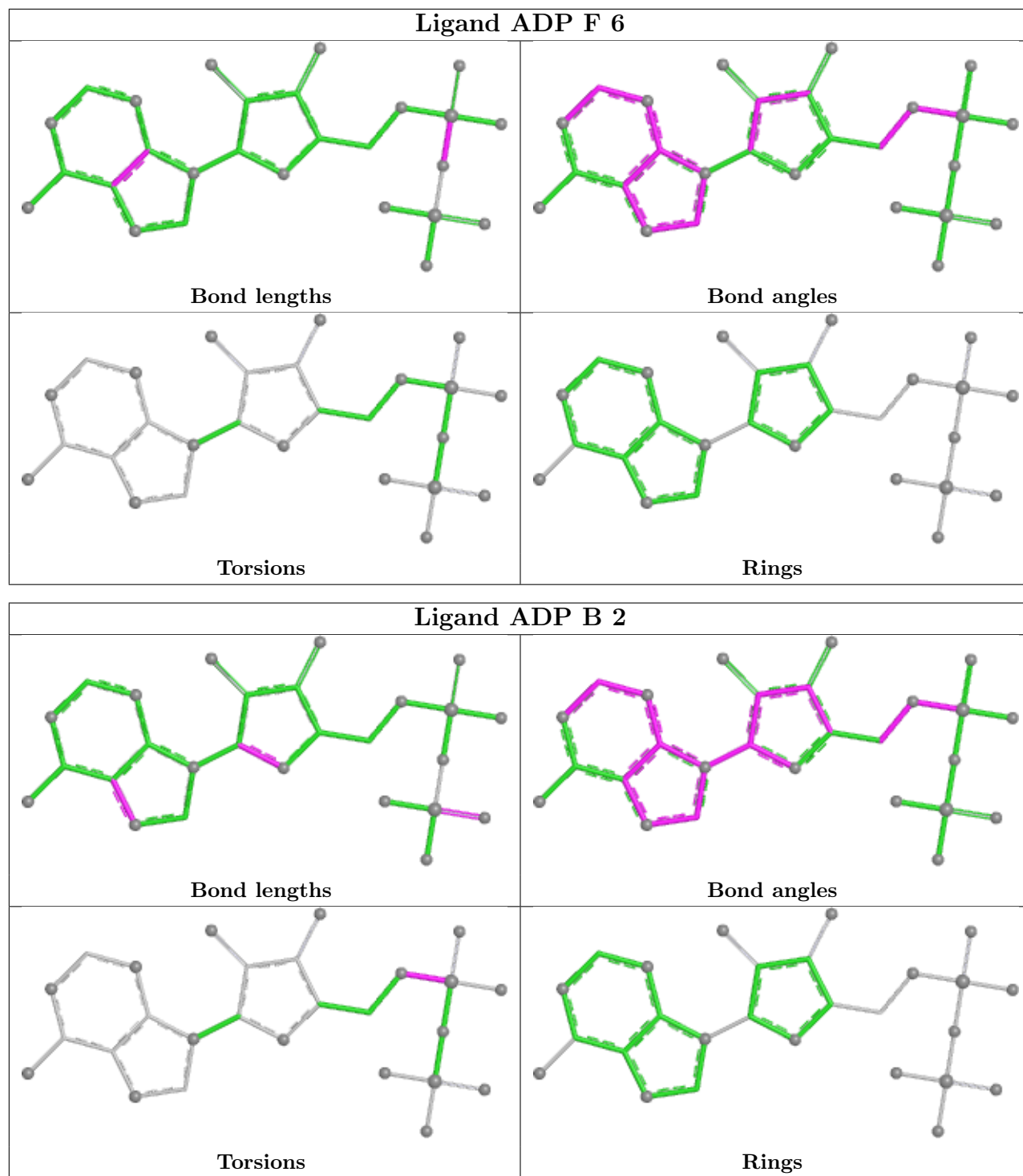


Ligand ADP K 10



Ligand ADP A 1





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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	M	6/13 (46%)	0.07	0 100 100	60, 67, 70, 143	0
1	N	7/13 (53%)	-0.43	0 100 100	53, 64, 110, 140	0
2	A	270/274 (98%)	-0.22	3 (1%) 78 60	25, 55, 147, 188	0
2	B	270/274 (98%)	-0.30	1 (0%) 88 78	25, 49, 123, 195	0
2	C	270/274 (98%)	0.01	8 (2%) 52 32	27, 67, 154, 200	0
2	D	270/274 (98%)	0.05	12 (4%) 39 22	32, 69, 151, 194	0
2	E	274/274 (100%)	-0.16	4 (1%) 72 52	25, 64, 131, 205	0
2	F	270/274 (98%)	-0.13	4 (1%) 72 52	26, 60, 131, 202	0
2	G	270/274 (98%)	-0.09	5 (1%) 66 45	25, 63, 129, 192	0
2	H	274/274 (100%)	-0.15	3 (1%) 78 60	26, 60, 135, 205	0
2	I	270/274 (98%)	-0.07	5 (1%) 66 45	25, 69, 153, 192	0
2	J	270/274 (98%)	-0.09	7 (2%) 57 36	27, 63, 136, 205	0
2	K	273/274 (99%)	-0.12	6 (2%) 62 41	25, 59, 150, 198	0
2	L	270/274 (98%)	0.41	25 (9%) 14 8	38, 119, 186, 205	0
All	All	3264/3314 (98%)	-0.07	83 (2%) 58 37	25, 64, 154, 205	0

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	467	ALA	6.9
2	G	551	GLU	4.1
2	L	444	ASN	4.0
2	L	386	CYS	3.7
2	D	549	THR	3.4
2	F	434	PRO	3.3
2	L	436	ASN	3.2
2	L	533	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
2	L	552	SER	3.1
2	L	503	ILE	3.0
2	G	550	ASP	2.9
2	D	550	ASP	2.9
2	L	441	MET	2.9
2	L	457	PHE	2.8
2	A	550	ASP	2.8
2	K	479	ASP	2.8
2	D	442	LEU	2.8
2	E	555	GLN	2.8
2	K	557	PHE	2.8
2	K	333	TYR	2.8
2	L	440	SER	2.8
2	D	402	PHE	2.7
2	L	450	LEU	2.7
2	L	553	GLY	2.7
2	J	309	GLU	2.7
2	G	487	TYR	2.6
2	L	542	PHE	2.6
2	G	492	LEU	2.6
2	L	434	PRO	2.6
2	L	538	ARG	2.6
2	H	309	GLU	2.5
2	J	348	PHE	2.5
2	L	488	PHE	2.5
2	L	466	LEU	2.5
2	L	469	LEU	2.5
2	D	557	PHE	2.5
2	E	558	ASN	2.5
2	I	540	GLN	2.5
2	K	495	ALA	2.4
2	C	550	ASP	2.4
2	H	550	ASP	2.4
2	J	549	THR	2.4
2	L	435	PRO	2.4
2	J	552	SER	2.4
2	L	447	ILE	2.4
2	L	492	LEU	2.4
2	D	412	PHE	2.4
2	F	556	PRO	2.4
2	J	548	CYS	2.4
2	C	436	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
2	C	402	PHE	2.3
2	C	556	PRO	2.3
2	I	494	ASN	2.3
2	F	549	THR	2.3
2	C	463	HIS	2.3
2	D	327	GLU	2.3
2	D	393	GLY	2.3
2	E	553	GLY	2.3
2	A	577	LEU	2.3
2	C	568	PHE	2.3
2	D	527	GLN	2.3
2	L	501	VAL	2.3
2	C	351	THR	2.2
2	G	399	LEU	2.2
2	D	558	ASN	2.2
2	C	398	ILE	2.2
2	D	352	ASN	2.2
2	F	495	ALA	2.2
2	J	554	GLU	2.2
2	I	550	ASP	2.2
2	L	568	PHE	2.1
2	I	507	HIS	2.1
2	I	308	THR	2.1
2	H	463	HIS	2.1
2	E	524	ILE	2.1
2	D	540	GLN	2.1
2	J	540	GLN	2.1
2	A	556	PRO	2.1
2	K	324	LYS	2.1
2	L	443	CYS	2.1
2	L	456	SER	2.1
2	B	548	CYS	2.1
2	K	550	ASP	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 oligosaccharides in this entry.

6.4 Ligands ⓘ

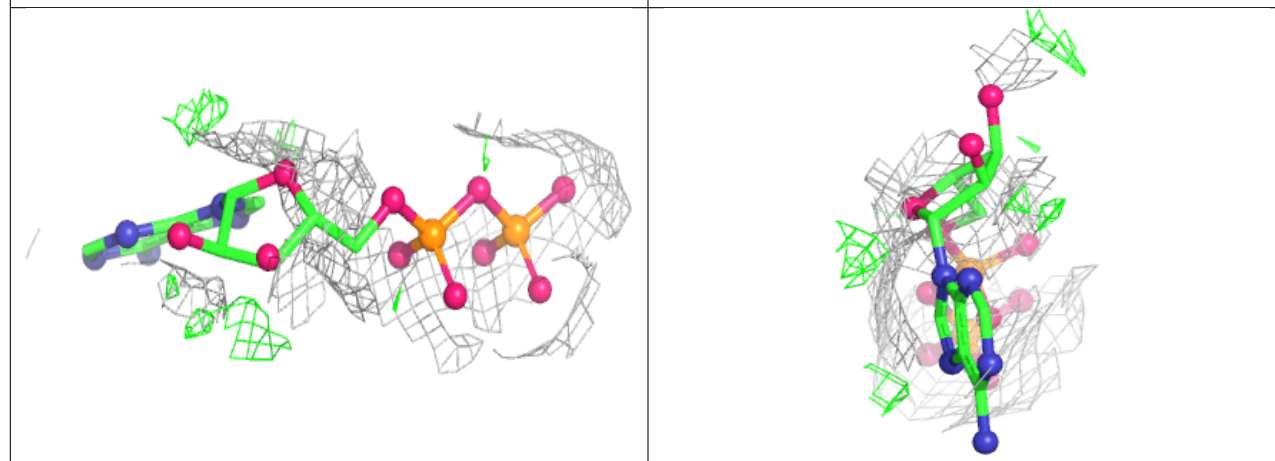
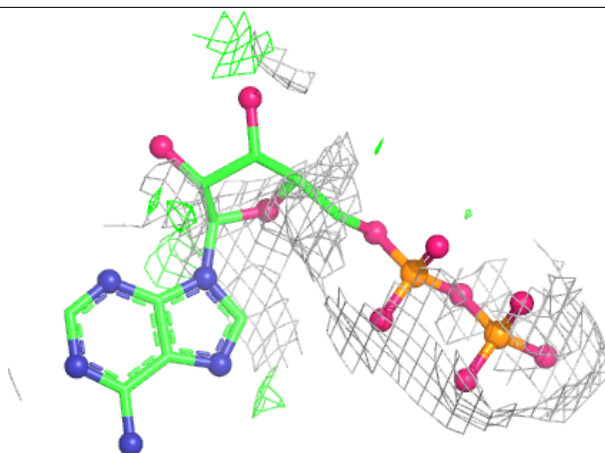
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	ADP	F	6	27/27	0.80	0.14	65,130,198,198	10
3	MG	I	29	1/1	0.81	0.12	55,55,55,55	0
5	ADP	D	4	27/27	0.82	0.16	81,119,162,162	10
5	ADP	L	11	27/27	0.87	0.13	84,142,198,198	0
4	CL	H	48	1/1	0.88	0.05	80,80,80,80	0
4	CL	B	42	1/1	0.89	0.08	73,73,73,73	0
5	ADP	E	5	27/27	0.90	0.16	77,105,195,195	10
5	ADP	C	3	27/27	0.90	0.10	70,80,100,100	0
5	ADP	H	8	27/27	0.90	0.14	70,94,123,123	0
5	ADP	J	9	27/27	0.90	0.14	89,126,182,182	10
5	ADP	B	2	27/27	0.90	0.12	55,69,88,88	0
5	ADP	G	7	27/27	0.91	0.11	58,70,90,90	0
5	ADP	A	1	27/27	0.92	0.11	31,65,66,66	0
3	MG	J	30	1/1	0.93	0.15	36,36,36,36	0
4	CL	A	41	1/1	0.93	0.13	70,70,70,70	0
3	MG	K	31	1/1	0.94	0.04	51,51,51,51	0
3	MG	E	25	1/1	0.94	0.09	30,30,30,30	0
5	ADP	K	10	27/27	0.95	0.10	67,74,133,133	10
3	MG	H	28	1/1	0.97	0.07	25,25,25,25	0
3	MG	D	24	1/1	0.97	0.08	50,50,50,50	0
3	MG	G	27	1/1	0.97	0.08	33,33,33,33	0
3	MG	B	22	1/1	0.98	0.04	25,25,25,25	0
3	MG	C	23	1/1	0.99	0.03	25,25,25,25	0
3	MG	A	21	1/1	0.99	0.06	25,25,25,25	0

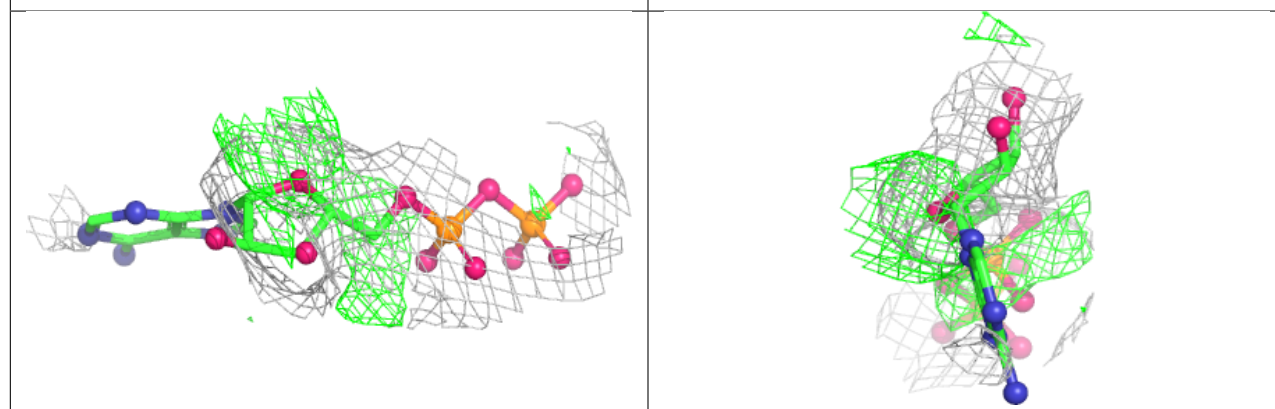
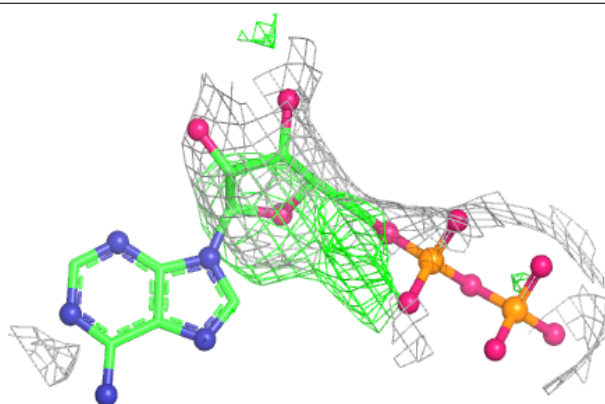
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around ADP F 6:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

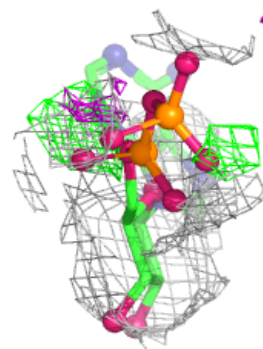
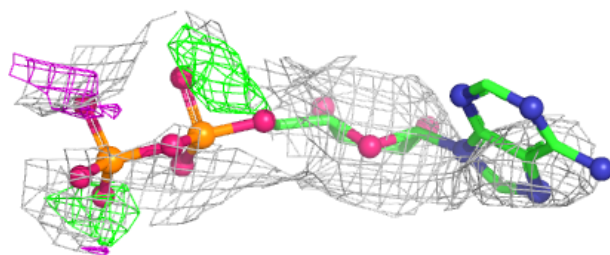
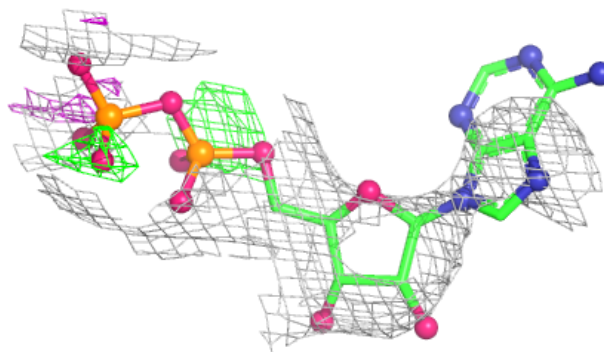
**Electron density around ADP D 4:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

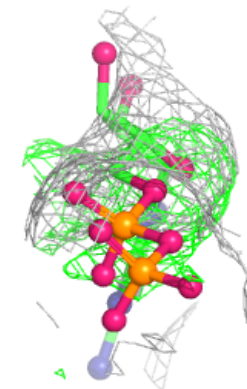
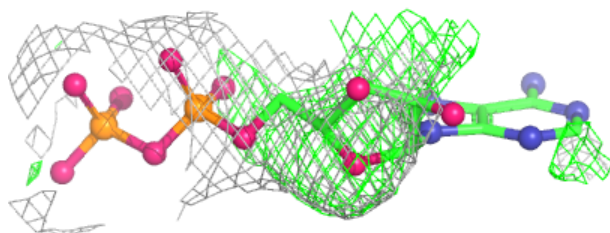
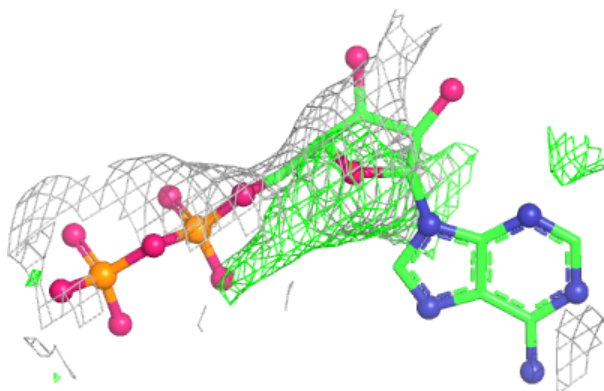


Electron density around ADP L 11:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

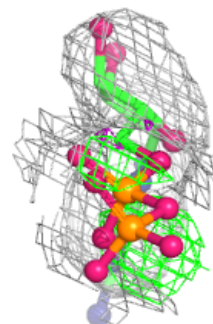
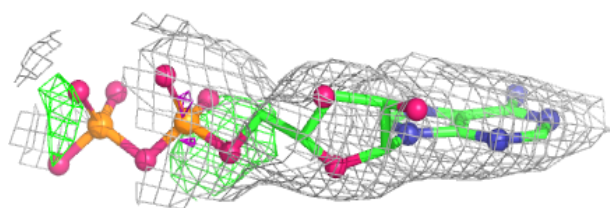
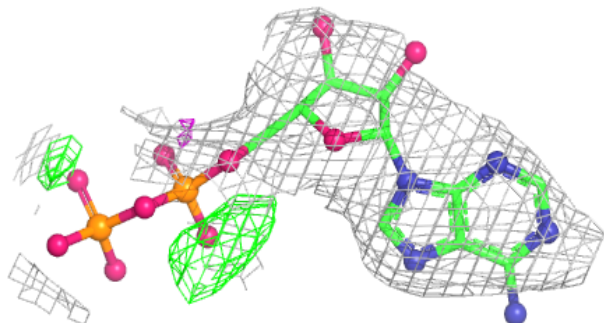
**Electron density around ADP E 5:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

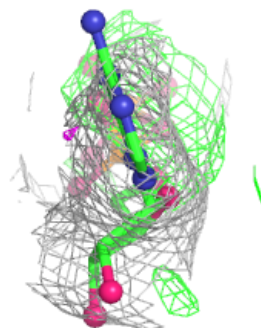
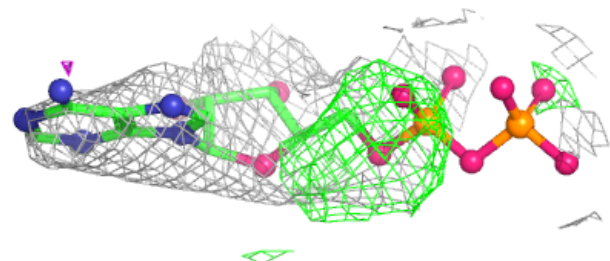
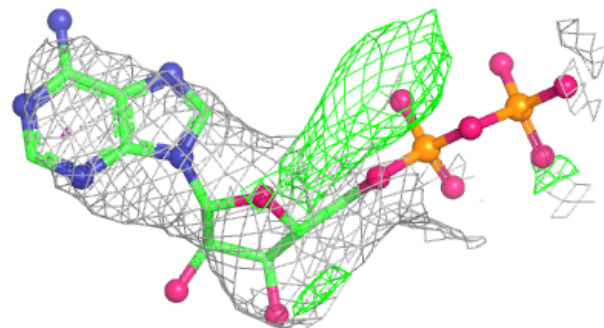


Electron density around ADP C 3:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

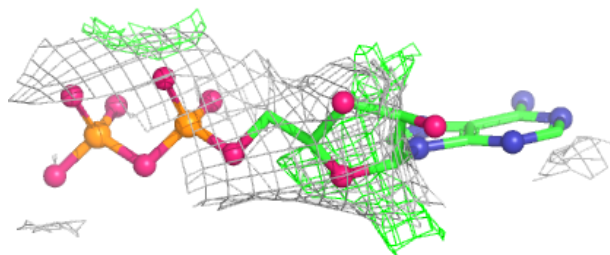
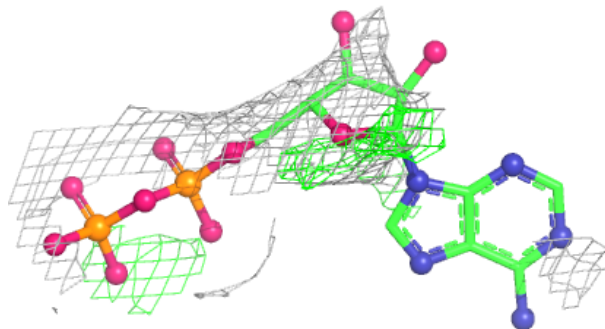
**Electron density around ADP H 8:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

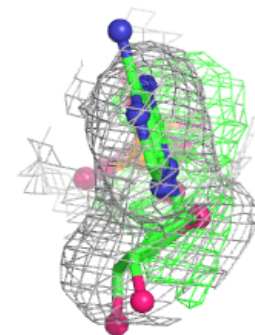
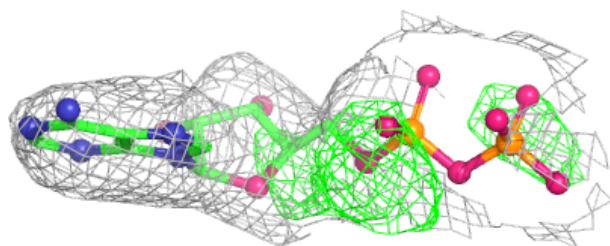
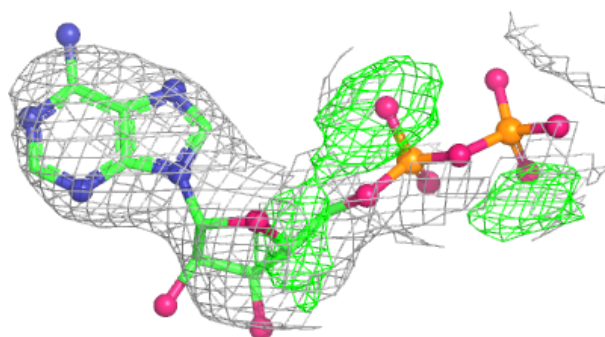


Electron density around ADP J 9:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

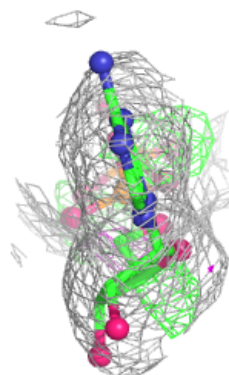
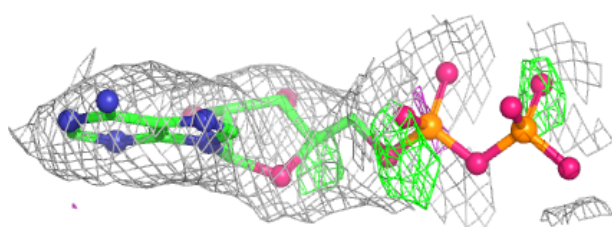
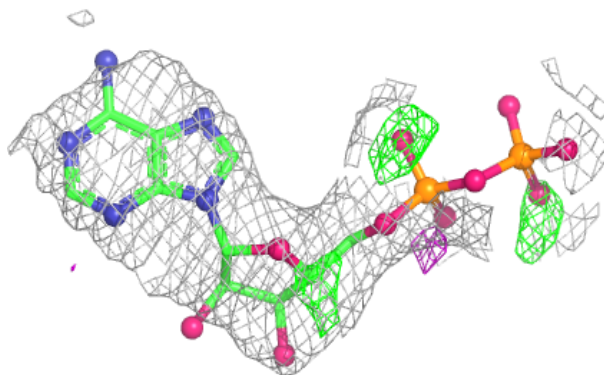
**Electron density around ADP B 2:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

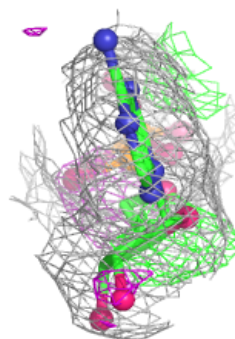
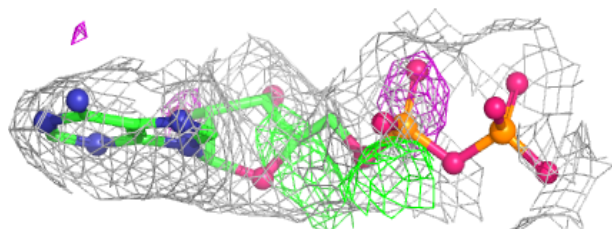
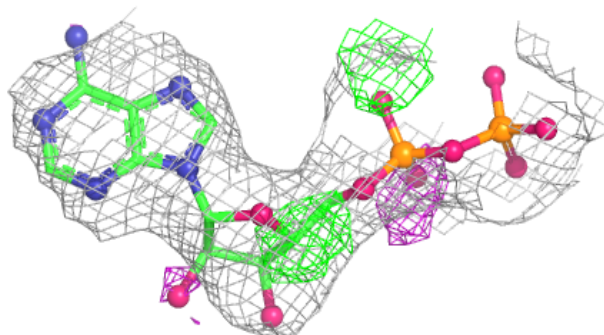


Electron density around ADP G 7:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

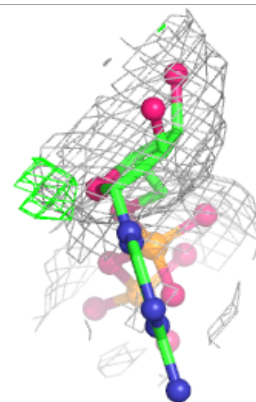
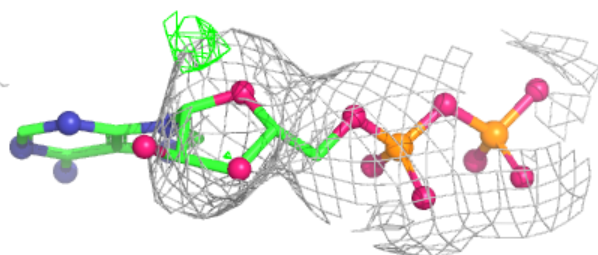
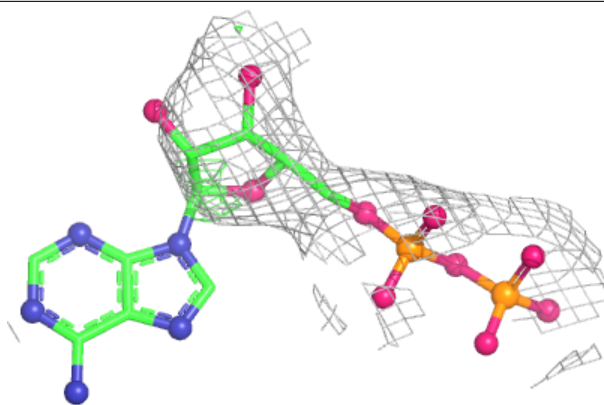
**Electron density around ADP A 1:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
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and green (positive)



Electron density around ADP K 10:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.