



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:22 AM UTC

PDB ID : 7WRX / pdb_00007wrx
Title : Structure of Deinococcus radiodurans HerA-ADP complex
Authors : Cheng, K.
Deposited on : 2022-01-27
Resolution : 3.40 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

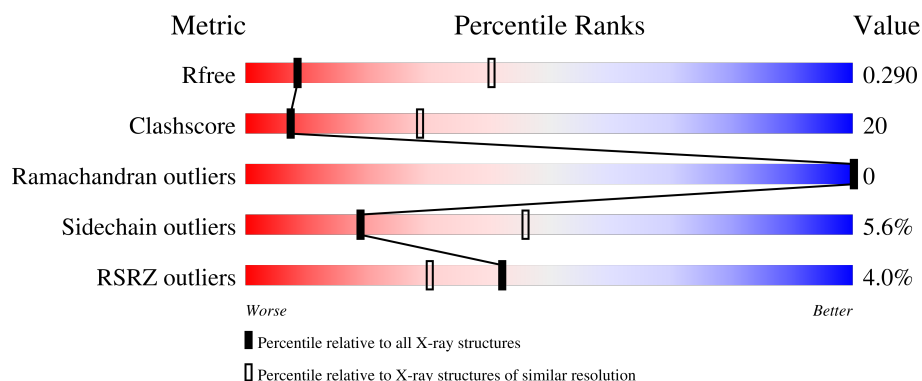
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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

Mol	Chain	Length	Quality of chain
1	A	618	5% 66% 28% • •
1	B	618	4% 59% 33% • 5%
1	C	618	4% 67% 27% • •
1	D	618	4% 67% 27% • •
1	E	618	3% 59% 34% • 5%

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Mol	Chain	Length	Quality of chain
1	F	618	
1	G	618	
1	H	618	
1	I	618	
1	J	618	
1	K	618	
1	L	618	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ADP	A	1001	-	-	X	-
3	ADP	E	1001	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 55302 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

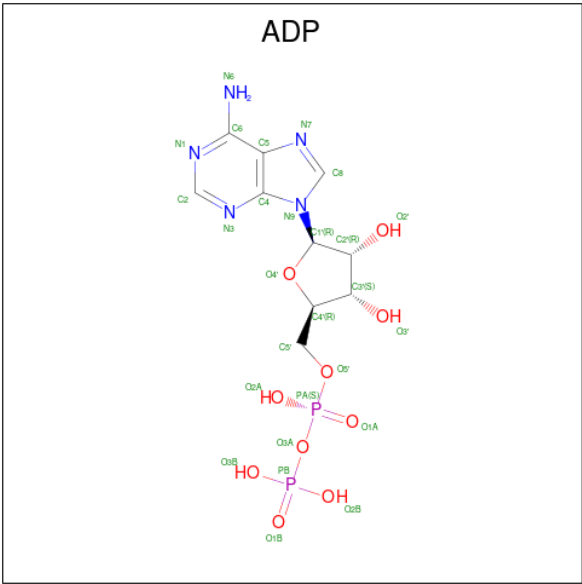
- Molecule 1 is a protein called HerA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	594	Total	C	N	O	S	0	0	0
			4591	2907	815	860	9			
1	A	591	Total	C	N	O	S	0	0	0
			4575	2897	812	857	9			
1	B	590	Total	C	N	O	S	0	0	0
			4567	2893	811	854	9			
1	C	594	Total	C	N	O	S	0	0	0
			4591	2907	815	860	9			
1	D	591	Total	C	N	O	S	0	0	0
			4575	2897	812	857	9			
1	E	590	Total	C	N	O	S	0	0	0
			4571	2896	811	855	9			
1	F	591	Total	C	N	O	S	0	0	0
			4575	2897	812	857	9			
1	G	594	Total	C	N	O	S	0	0	0
			4591	2907	815	860	9			
1	I	594	Total	C	N	O	S	0	0	0
			4591	2907	815	860	9			
1	J	590	Total	C	N	O	S	0	0	0
			4567	2893	811	854	9			
1	K	594	Total	C	N	O	S	0	0	0
			4591	2907	815	860	9			
1	L	594	Total	C	N	O	S	0	0	0
			4591	2907	815	860	9			

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	H	1	Total	Mg	0	0
			1	1		
2	D	1	Total	Mg	0	0
			1	1		

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).

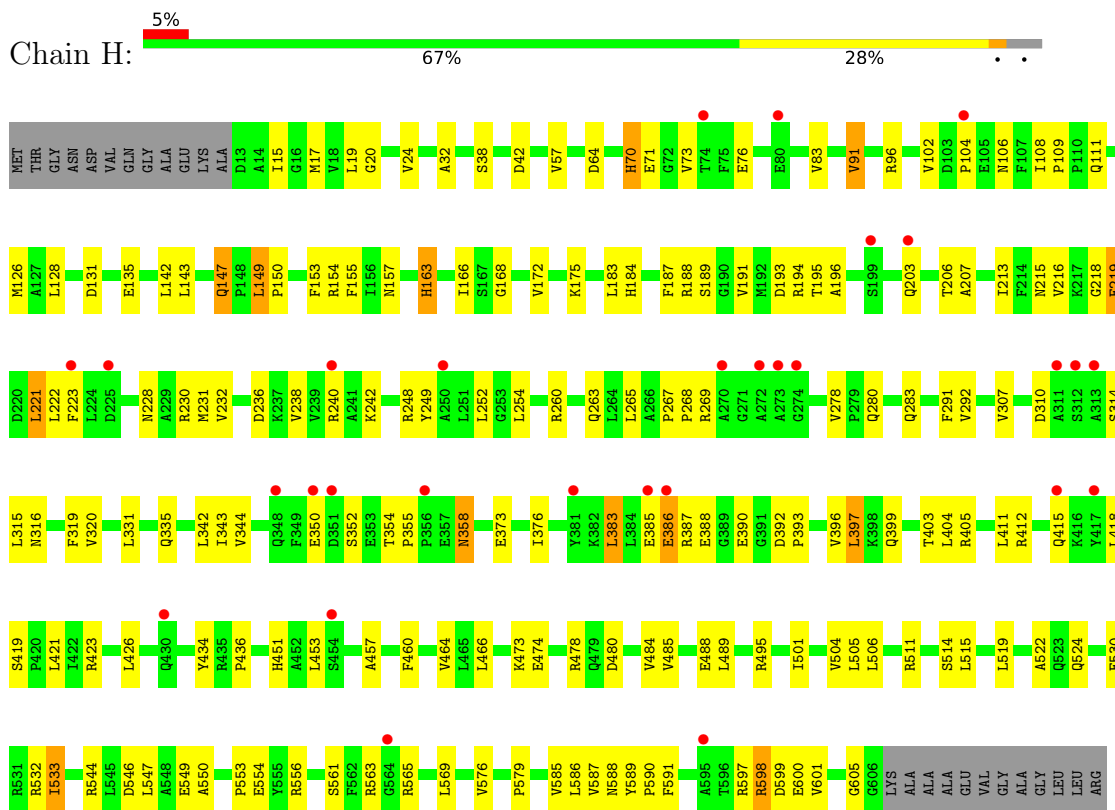


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	H	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	F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

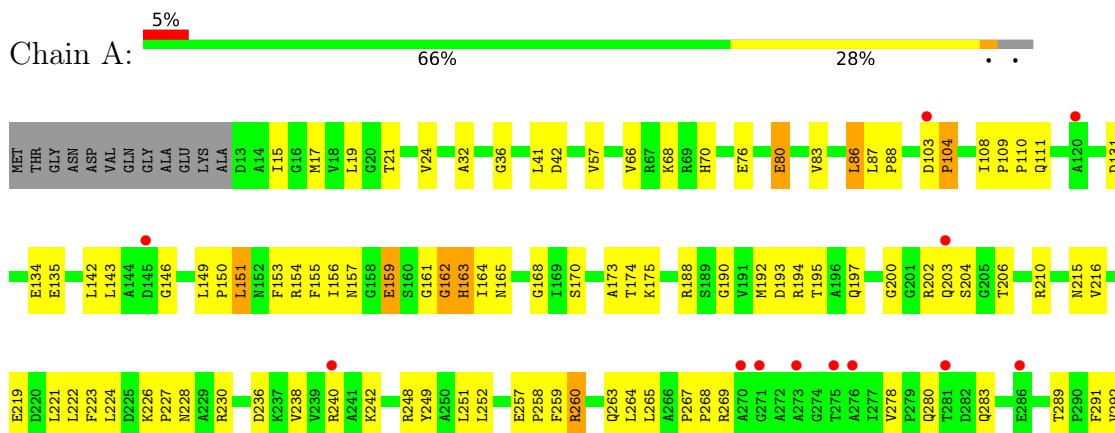
3 Residue-property plots

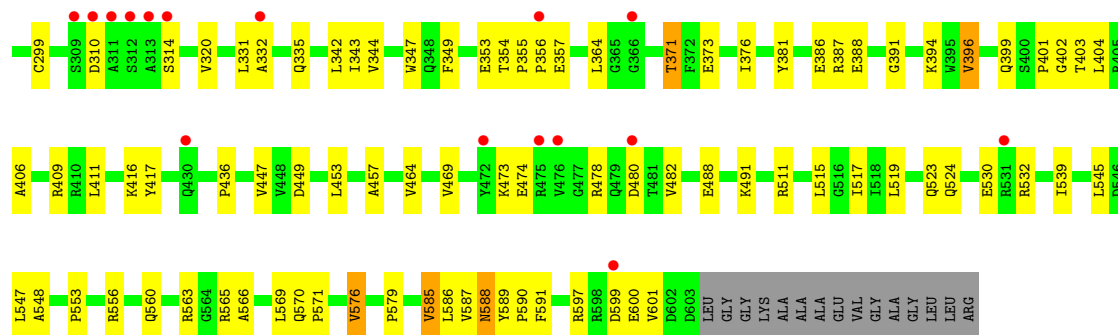
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: HerA

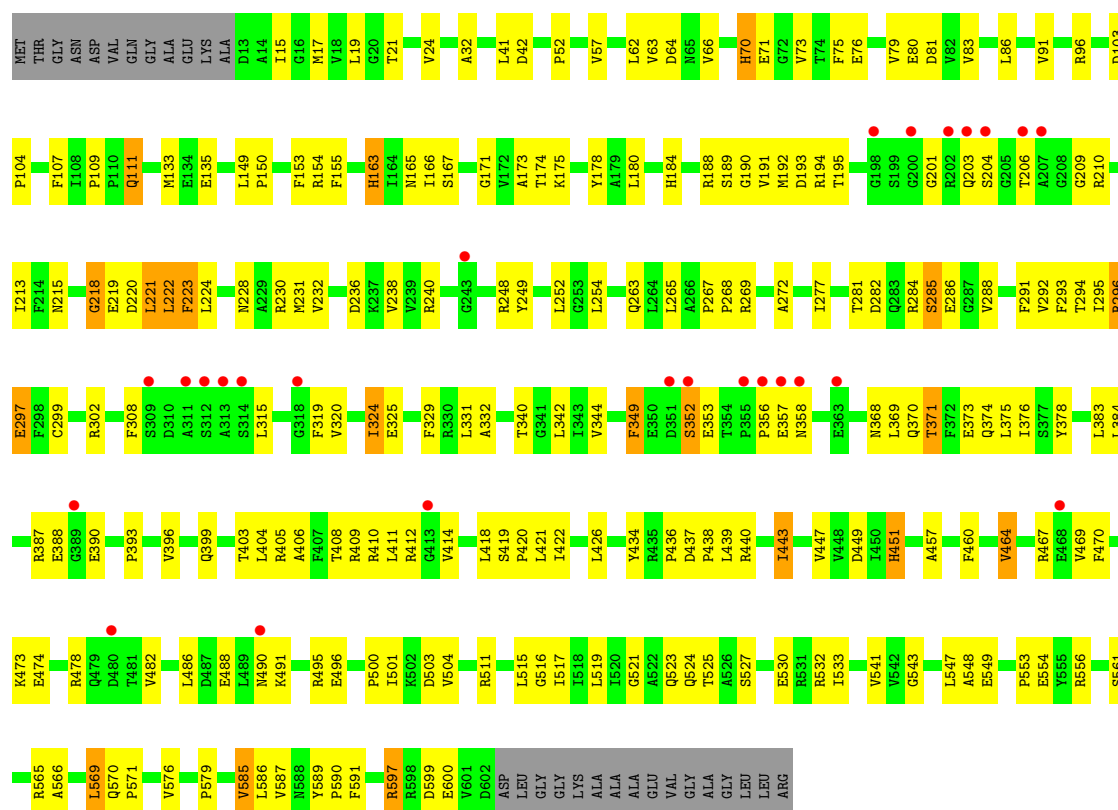


• Molecule 1: HerA

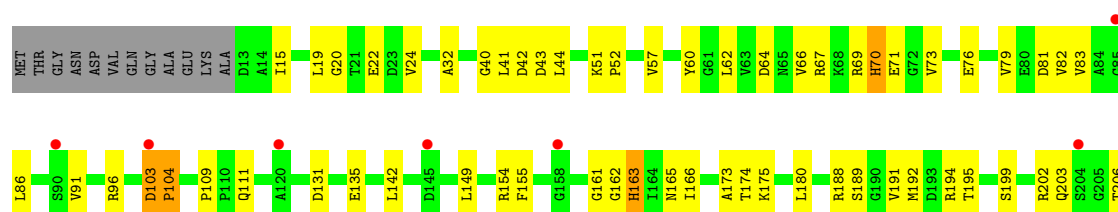


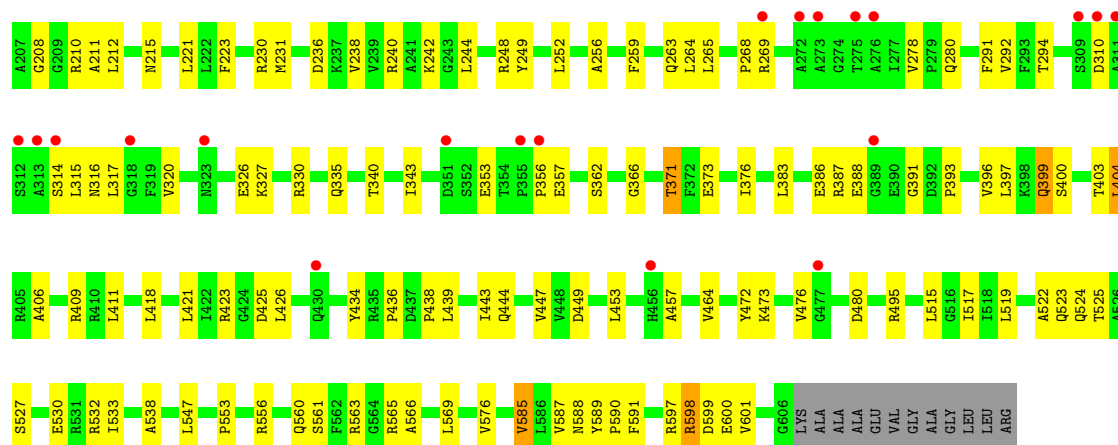


• Molecule 1: HerA

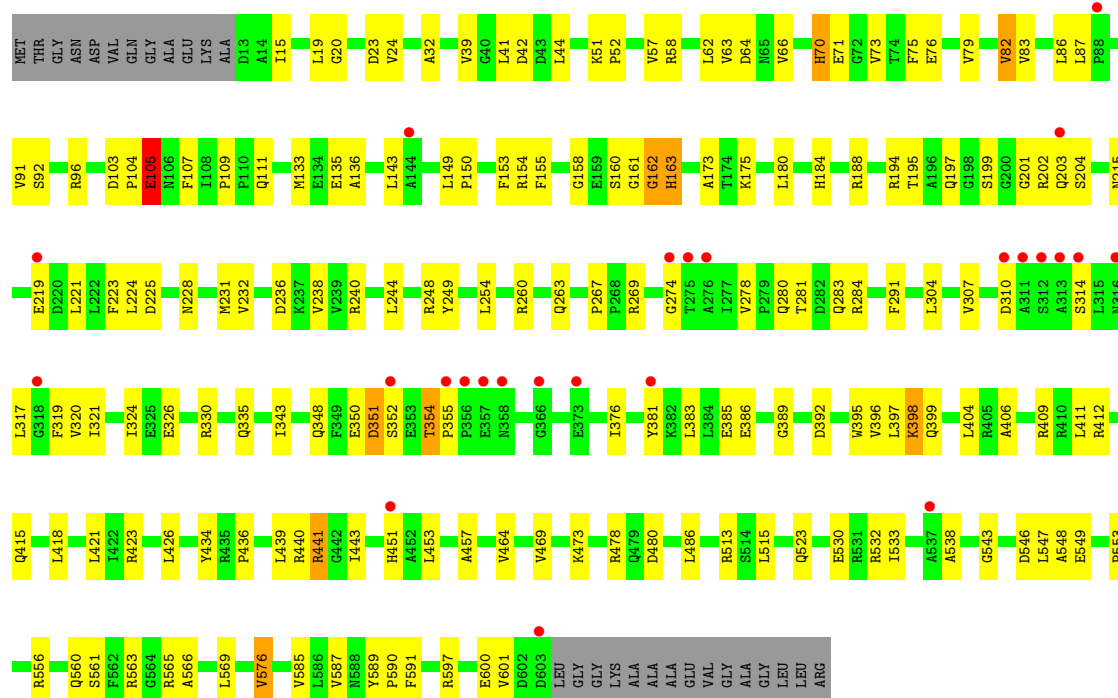


• Molecule 1: HerA

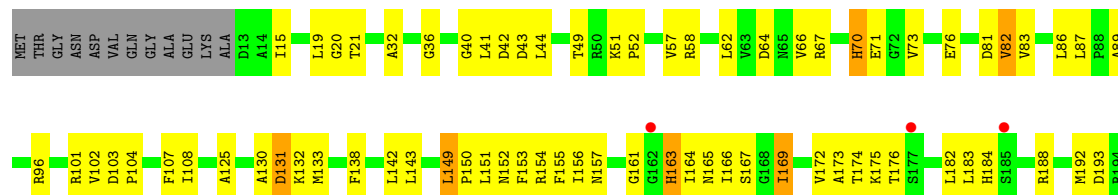


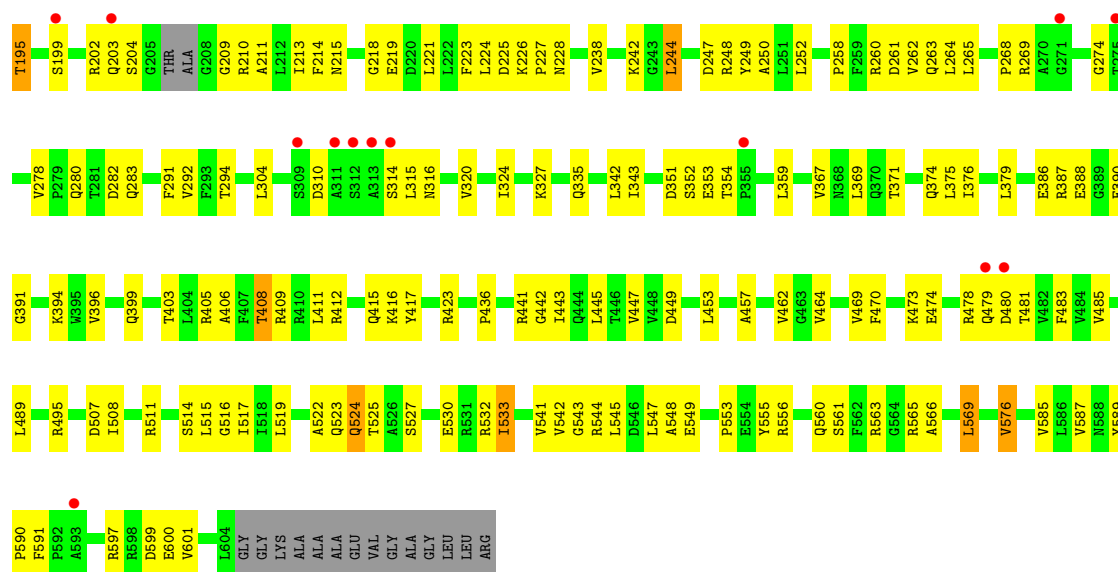


• Molecule 1: HerA



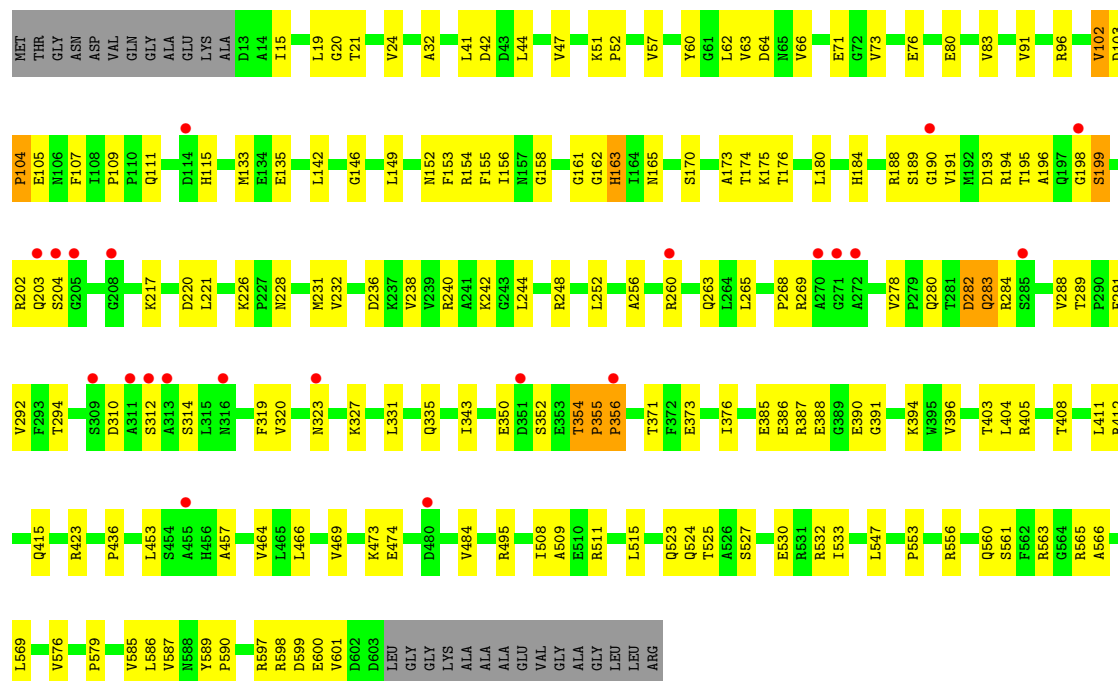
• Molecule 1: HerA





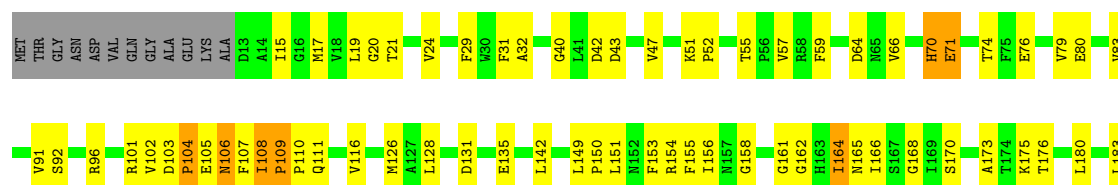
• Molecule 1: HerA

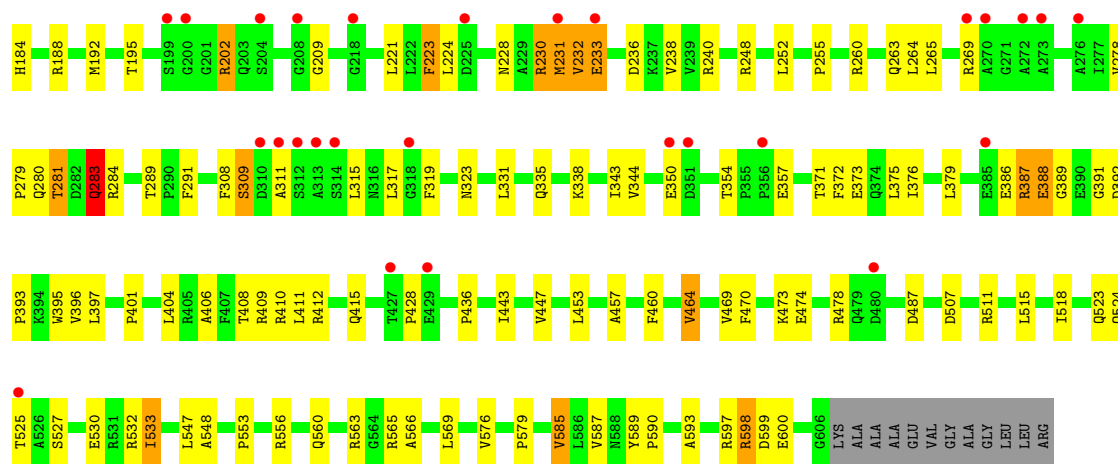
Chain F: 4% 67% 27% . .



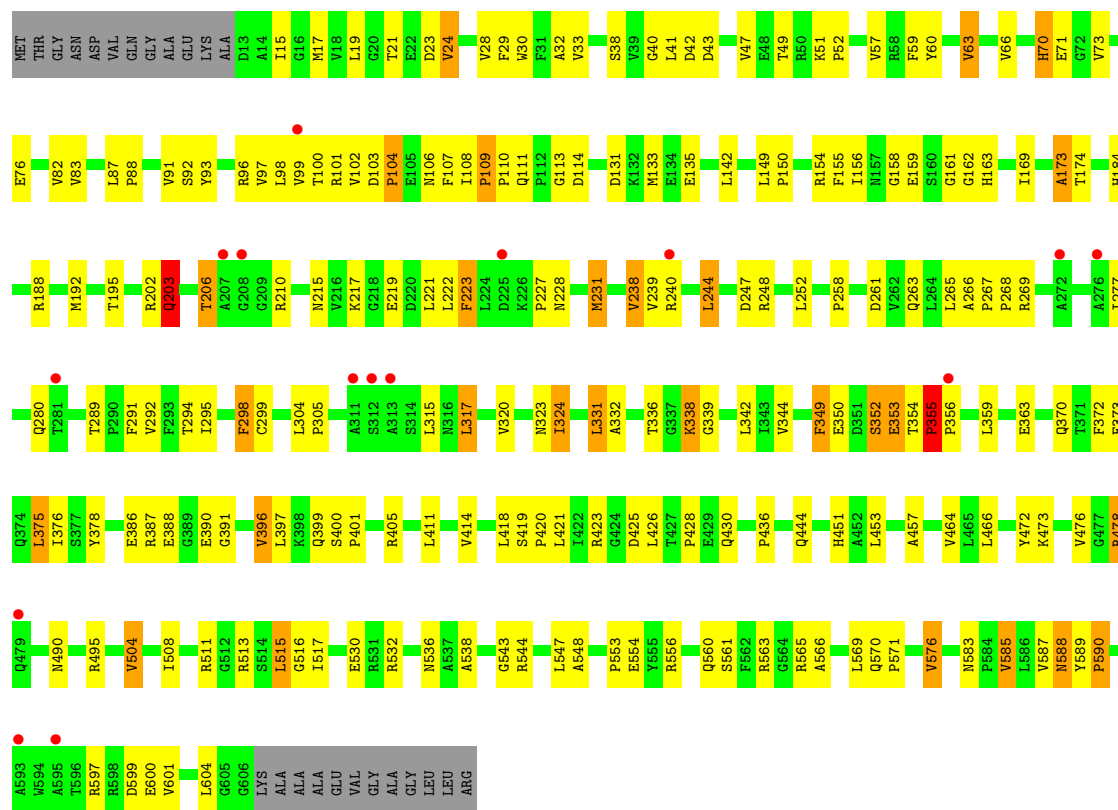
• Molecule 1: HerA

Chain G: 4% 66% 26% . .

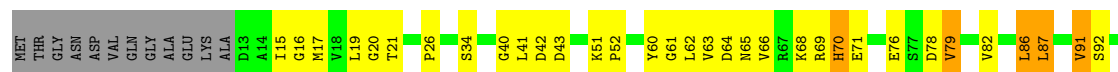


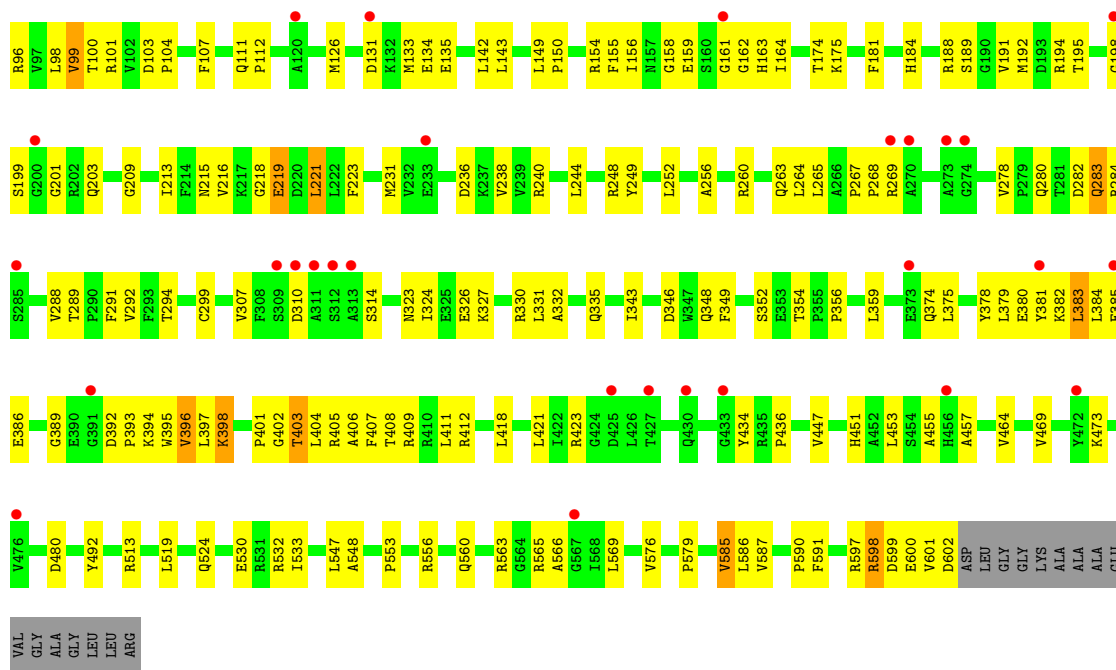


• Molecule 1: HerA

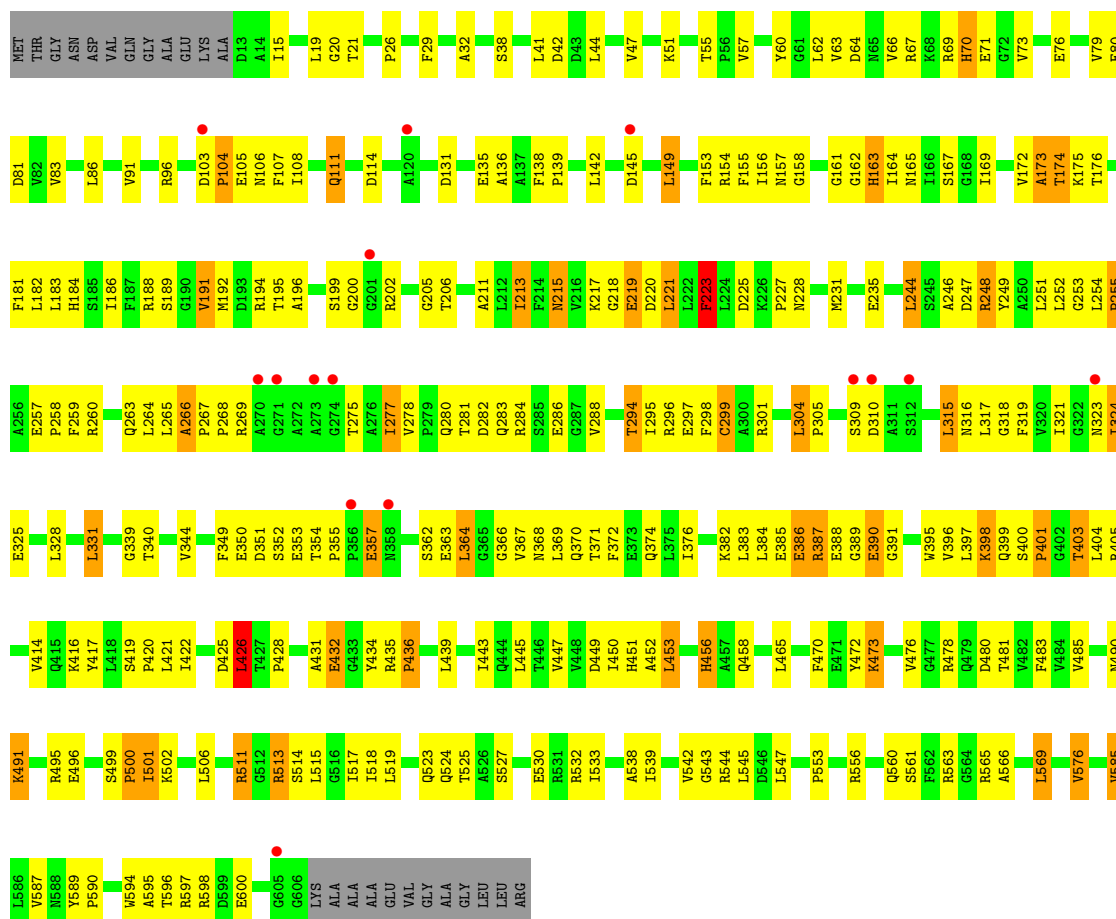


• Molecule 1: HerA

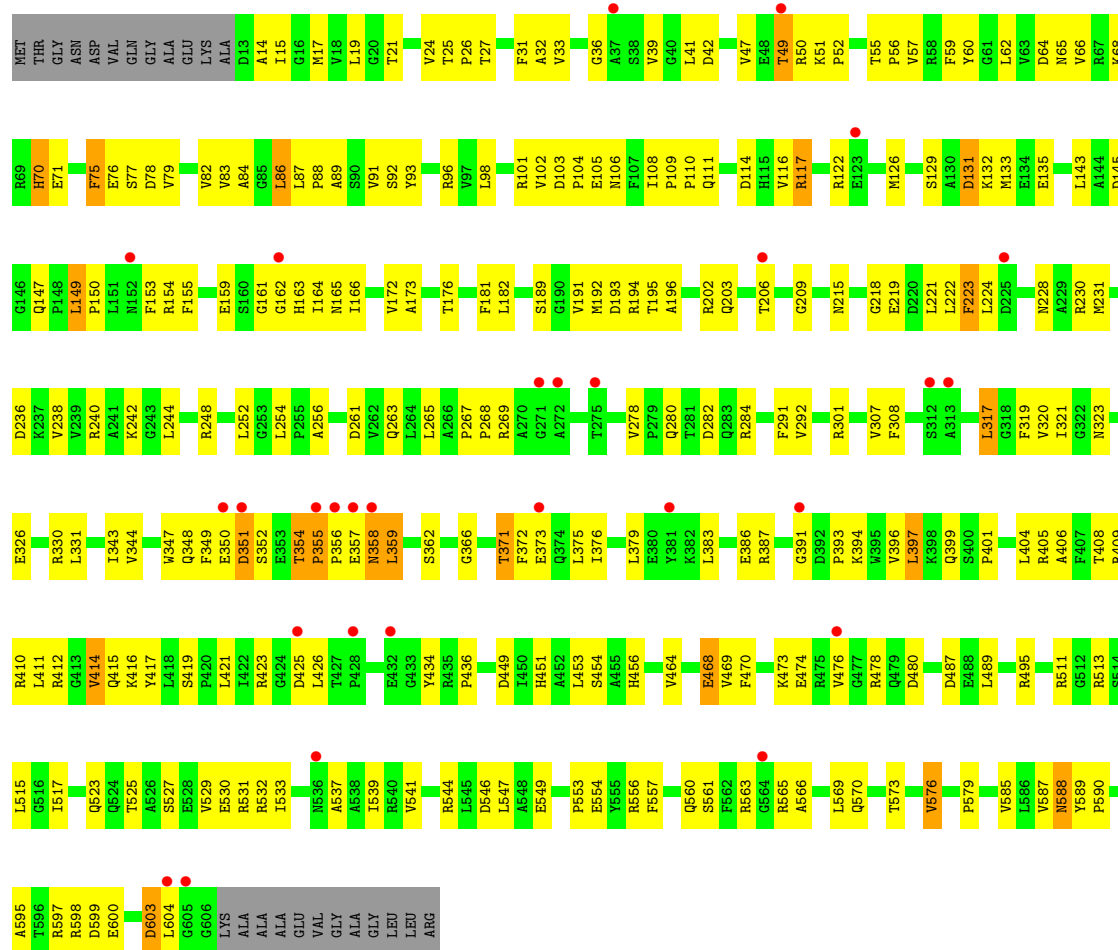




• Molecule 1: HerA



● Molecule 1: HerA



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	106.01Å 202.87Å 411.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 3.40 10.00 – 3.40	Depositor EDS
% Data completeness (in resolution range)	97.6 (10.00-3.40) 93.4 (10.00-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.73 (at 3.37Å)	Xtriage
Refinement program	PHENIX 1.11.1 _2575	Depositor
R, R_{free}	0.276 , 0.291 0.276 , 0.290	Depositor DCC
R_{free} test set	6066 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	80.1	Xtriage
Anisotropy	0.431	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 34.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	55302	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.98% 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: 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	A	0.45	2/4670 (0.0%)	0.67	7/6338 (0.1%)
1	B	0.64	0/4662	0.96	10/6327 (0.2%)
1	C	0.42	1/4686 (0.0%)	0.67	7/6359 (0.1%)
1	D	0.36	0/4670	0.64	9/6338 (0.1%)
1	E	0.45	0/4665	0.72	0/6329
1	F	0.53	4/4670 (0.1%)	0.81	10/6338 (0.2%)
1	G	0.39	2/4686 (0.0%)	0.69	15/6359 (0.2%)
1	H	0.37	0/4686	0.65	4/6359 (0.1%)
1	I	0.82	3/4686 (0.1%)	1.18	12/6359 (0.2%)
1	J	0.37	0/4662	0.71	7/6327 (0.1%)
1	K	0.82	2/4686 (0.0%)	1.25	28/6359 (0.4%)
1	L	0.48	3/4686 (0.1%)	0.79	10/6359 (0.2%)
All	All	0.53	17/56115 (0.0%)	0.84	119/76151 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1
1	G	0	1
All	All	0	2

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	356	PRO	N-CA	17.36	1.70	1.47
1	C	104	PRO	N-CA	17.09	1.69	1.47
1	F	355	PRO	N-CA	11.73	1.70	1.46
1	L	355	PRO	N-CA	10.72	1.68	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	354	THR	C-N	10.45	1.45	1.33
1	K	436	PRO	N-CD	-10.44	1.33	1.47
1	A	150	PRO	N-CD	10.37	1.62	1.47
1	L	354	THR	C-N	10.33	1.45	1.33
1	F	355	PRO	C-N	10.31	1.45	1.34
1	L	278	VAL	C-O	7.82	1.29	1.24
1	G	388	GLU	CA-C	7.42	1.62	1.52
1	I	355	PRO	C-N	7.17	1.50	1.33
1	G	109	PRO	C-O	-6.59	1.19	1.24
1	I	109	PRO	C-O	-5.95	1.17	1.24
1	A	278	VAL	C-O	-5.89	1.20	1.24
1	I	590	PRO	C-O	-5.23	1.17	1.23
1	K	401	PRO	C-O	-5.06	1.17	1.24

All (119) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	355	PRO	CA-C-N	18.83	139.46	119.87
1	F	355	PRO	C-N-CA	18.83	139.46	119.87
1	L	354	THR	CA-C-N	18.42	139.36	120.38
1	L	354	THR	C-N-CA	18.42	139.36	120.38
1	F	354	THR	CA-C-N	18.30	139.23	120.38
1	F	354	THR	C-N-CA	18.30	139.23	120.38
1	C	103	ASP	CA-C-N	15.16	138.79	119.84
1	C	103	ASP	C-N-CA	15.16	138.79	119.84
1	K	436	PRO	N-CA-CB	-12.52	94.84	103.23
1	J	283	GLN	N-CA-C	11.54	123.86	111.28
1	C	104	PRO	N-CA-C	-11.42	88.94	112.47
1	B	224	LEU	N-CA-C	-9.78	101.34	113.28
1	K	426	LEU	N-CA-C	8.99	122.92	110.24
1	L	355	PRO	CA-N-CD	-8.90	99.53	112.00
1	D	202	ARG	N-CA-C	-8.81	101.65	111.07
1	F	356	PRO	CA-N-CD	-8.77	99.72	112.00
1	C	104	PRO	CA-N-CD	-8.73	99.77	112.00
1	F	355	PRO	CA-N-CD	-8.49	100.11	112.00
1	G	283	GLN	CA-C-N	-8.36	110.86	123.07
1	G	283	GLN	C-N-CA	-8.36	110.86	123.07
1	B	352	SER	N-CA-C	-8.20	102.84	113.17
1	A	104	PRO	N-CA-C	-8.11	95.76	112.47
1	I	355	PRO	CA-C-N	7.89	134.45	120.88
1	I	355	PRO	C-N-CA	7.89	134.45	120.88
1	L	224	LEU	N-CA-C	-7.73	103.87	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	201	GLY	N-CA-C	7.72	121.99	112.64
1	A	150	PRO	N-CA-CB	7.39	109.86	103.36
1	I	104	PRO	N-CA-C	-7.26	97.52	112.47
1	G	109	PRO	CB-CA-C	-7.11	104.48	111.17
1	K	206	THR	CB-CA-C	-7.04	99.11	110.79
1	J	598	ARG	N-CA-C	6.99	118.55	111.07
1	A	162	GLY	CA-C-N	6.99	136.14	122.73
1	A	162	GLY	C-N-CA	6.99	136.14	122.73
1	H	460	PHE	N-CA-C	-6.98	103.28	111.03
1	K	478	ARG	CA-C-N	-6.88	109.27	122.06
1	K	478	ARG	C-N-CA	-6.88	109.27	122.06
1	G	387	ARG	CB-CA-C	6.84	122.19	111.72
1	K	104	PRO	N-CA-C	-6.82	98.42	112.47
1	H	598	ARG	N-CA-C	6.79	118.69	111.28
1	B	358	ASN	N-CA-C	-6.76	97.26	108.34
1	D	202	ARG	CA-C-N	6.67	132.39	122.99
1	D	202	ARG	C-N-CA	6.67	132.39	122.99
1	G	281	THR	CB-CA-C	-6.65	100.47	109.71
1	G	232	VAL	N-CA-C	-6.53	104.49	110.82
1	K	436	PRO	CA-N-CD	6.42	120.99	112.00
1	K	174	THR	CA-CB-OG1	-6.35	100.08	109.60
1	J	283	GLN	N-CA-CB	-6.34	100.80	110.12
1	H	605	GLY	N-CA-C	6.25	120.55	112.68
1	L	278	VAL	O-C-N	-6.18	117.80	121.69
1	H	106	ASN	N-CA-C	-6.13	98.53	108.52
1	C	598	ARG	N-CA-C	6.08	117.58	111.07
1	G	230	ARG	N-CA-C	6.06	120.51	113.18
1	G	109	PRO	N-CA-C	6.03	117.03	110.58
1	K	436	PRO	CB-CA-C	-5.99	105.95	111.40
1	K	500	PRO	CB-CA-C	-5.94	103.64	112.55
1	G	104	PRO	N-CA-C	-5.94	100.24	112.47
1	G	598	ARG	N-CA-C	5.91	117.39	111.07
1	I	109	PRO	CB-CA-C	-5.85	103.78	110.92
1	C	399	GLN	N-CA-C	-5.82	101.86	110.48
1	D	75	PHE	CB-CA-C	5.82	118.57	109.84
1	K	478	ARG	CA-C-O	-5.79	112.89	119.78
1	I	590	PRO	CB-CA-C	-5.79	103.65	111.12
1	B	438	PRO	N-CA-C	-5.67	106.14	113.57
1	K	266	ALA	CA-C-N	5.65	123.73	119.66
1	K	266	ALA	C-N-CA	5.65	123.73	119.66
1	B	218	GLY	CA-C-N	5.61	130.10	122.07
1	B	218	GLY	C-N-CA	5.61	130.10	122.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	268	PRO	N-CA-C	5.60	122.80	112.33
1	I	203	GLN	CA-C-N	-5.57	115.14	122.99
1	I	203	GLN	C-N-CA	-5.57	115.14	122.99
1	I	173	ALA	CA-C-N	-5.52	113.73	122.23
1	I	173	ALA	C-N-CA	-5.52	113.73	122.23
1	G	389	GLY	N-CA-C	5.51	126.25	113.18
1	L	355	PRO	N-CD-CG	5.51	111.46	103.20
1	K	390	GLU	CB-CA-C	5.50	120.21	110.85
1	I	338	LYS	CA-C-N	5.49	125.32	120.10
1	I	338	LYS	C-N-CA	5.49	125.32	120.10
1	K	598	ARG	N-CA-C	5.48	116.94	111.07
1	K	426	LEU	N-CA-CB	-5.47	100.99	109.69
1	G	309	SER	CB-CA-C	-5.44	103.08	112.44
1	K	253	GLY	N-CA-C	-5.44	107.52	115.63
1	G	388	GLU	CA-C-O	5.43	128.28	120.51
1	B	349	PHE	CB-CA-C	5.42	119.72	111.70
1	L	351	ASP	N-CA-CB	-5.41	100.28	111.36
1	K	389	GLY	N-CA-C	-5.40	108.19	115.21
1	B	315	LEU	N-CA-C	5.35	116.93	108.96
1	J	398	LYS	N-CA-C	5.35	118.57	111.30
1	A	150	PRO	CA-N-CD	-5.33	104.54	112.00
1	K	173	ALA	N-CA-C	-5.30	102.00	109.96
1	K	398	LYS	N-CA-C	-5.29	104.09	111.39
1	K	432	GLU	CA-C-N	5.29	125.82	120.00
1	K	432	GLU	C-N-CA	5.29	125.82	120.00
1	B	220	ASP	N-CA-C	-5.29	107.20	113.97
1	D	202	ARG	O-C-N	5.26	127.49	122.07
1	L	358	ASN	N-CA-C	-5.26	102.50	110.24
1	F	220	ASP	N-CA-C	-5.26	106.88	113.72
1	K	255	PRO	CB-CA-C	-5.26	104.09	110.98
1	J	396	VAL	N-CA-C	-5.23	99.72	107.51
1	G	283	GLN	N-CA-CB	5.21	118.08	110.47
1	B	356	PRO	N-CA-C	-5.20	106.31	113.53
1	K	260	ARG	CA-C-N	-5.19	115.46	123.14
1	K	260	ARG	C-N-CA	-5.19	115.46	123.14
1	K	387	ARG	CB-CA-C	-5.14	104.74	112.09
1	F	283	GLN	CA-C-N	-5.12	115.56	123.14
1	F	283	GLN	C-N-CA	-5.12	115.56	123.14
1	D	105	GLU	CA-C-N	5.12	130.22	123.05
1	D	105	GLU	C-N-CA	5.12	130.22	123.05
1	G	311	ALA	N-CA-CB	-5.12	104.12	111.70
1	A	159	GLU	CB-CA-C	-5.08	103.14	110.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	223	PHE	CA-CB-CG	5.06	118.86	113.80
1	F	104	PRO	N-CA-C	-5.05	107.46	114.27
1	J	398	LYS	N-CA-CB	-5.05	104.40	111.62
1	A	259	PHE	CB-CA-C	5.02	117.73	109.90
1	C	356	PRO	N-CA-C	-5.02	106.56	113.53
1	D	162	GLY	CA-C-N	5.01	133.45	122.82
1	D	162	GLY	C-N-CA	5.01	133.45	122.82
1	L	117	ARG	N-CA-C	5.01	116.81	109.24
1	L	356	PRO	N-CA-C	-5.00	108.20	114.20
1	I	206	THR	N-CA-C	-5.00	107.35	113.50

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	439	LEU	Mainchain
1	G	231	MET	Mainchain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4575	0	4570	176	1
1	B	4567	0	4566	210	3
1	C	4591	0	4587	158	2
1	D	4575	0	4569	175	1
1	E	4571	0	4568	212	5
1	F	4575	0	4570	140	0
1	G	4591	0	4587	153	0
1	H	4591	0	4587	172	1
1	I	4591	0	4587	220	0
1	J	4567	0	4566	222	1
1	K	4591	0	4587	338	1
1	L	4591	0	4587	239	1
2	D	1	0	0	0	0
2	H	1	0	0	0	0
3	A	27	0	12	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	27	0	12	6	0
3	C	27	0	12	3	0
3	D	27	0	12	3	0
3	E	27	0	12	15	0
3	F	27	0	12	3	0
3	G	27	0	12	2	0
3	H	27	0	12	1	0
3	I	27	0	12	0	0
3	J	27	0	12	4	0
3	K	27	0	12	6	0
3	L	27	0	12	1	0
All	All	55302	0	55075	2250	8

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 20.

All (2250) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:355:PRO:N	1:F:355:PRO:CA	1.70	1.45
1:C:104:PRO:N	1:C:104:PRO:CA	1.69	1.45
1:F:356:PRO:N	1:F:356:PRO:CA	1.70	1.36
1:L:354:THR:OG1	1:L:355:PRO:HD2	1.21	1.35
1:I:87:LEU:HD12	1:I:88:PRO:CD	1.54	1.35
1:L:355:PRO:N	1:L:355:PRO:CA	1.68	1.33
1:K:192:MET:O	1:K:196:ALA:HB2	1.23	1.31
1:I:87:LEU:CD1	1:I:88:PRO:HD2	1.63	1.25
1:E:175:LYS:NZ	1:E:523:GLN:C	1.94	1.23
1:J:396:VAL:CG2	1:J:404:LEU:HD11	1.68	1.22
1:I:41:LEU:O	1:I:63:VAL:HG12	1.34	1.19
1:K:473:LYS:HG2	1:K:517:ILE:HG12	1.19	1.19
1:J:282:ASP:CB	1:K:202:ARG:HH12	1.56	1.16
1:L:354:THR:OG1	1:L:355:PRO:CD	1.93	1.15
1:B:396:VAL:HG23	1:B:404:LEU:HD11	1.21	1.15
1:I:42:ASP:OD1	1:I:565:ARG:NH1	1.81	1.13
1:J:282:ASP:HB3	1:K:202:ARG:HH12	1.03	1.10
1:G:155:PHE:HA	1:G:161:GLY:HA3	1.12	1.10
1:D:82:VAL:HG22	1:D:87:LEU:HD22	1.25	1.09
1:J:455:ALA:HB2	1:K:511:ARG:HD2	1.31	1.09
1:K:473:LYS:HG2	1:K:517:ILE:CG1	1.83	1.08
1:B:219:GLU:HA	1:B:222:LEU:HD11	1.34	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:103:ASP:HB3	1:D:104:PRO:CD	1.83	1.08
1:J:231:MET:HE1	1:J:256:ALA:HB1	1.35	1.08
1:J:354:THR:HG21	1:J:381:TYR:CE2	1.88	1.08
1:I:142:LEU:O	1:I:588:ASN:ND2	1.86	1.06
1:L:473:LYS:NZ	1:L:480:ASP:O	1.87	1.06
1:L:87:LEU:HD12	1:L:88:PRO:CD	1.85	1.06
1:H:223:PHE:CD1	1:H:601:VAL:HG21	1.91	1.06
1:A:155:PHE:CD2	1:A:579:PRO:HG2	1.90	1.05
1:F:57:VAL:HA	1:F:104:PRO:HG2	1.37	1.05
1:K:472:TYR:CE1	1:K:476:VAL:HG11	1.90	1.05
1:K:490:ASN:OD1	1:K:491:LYS:N	1.89	1.05
1:C:231:MET:HE1	1:C:256:ALA:HB1	1.33	1.05
1:C:155:PHE:HA	1:C:161:GLY:HA3	1.38	1.04
1:B:219:GLU:HA	1:B:222:LEU:CD1	1.87	1.04
1:L:87:LEU:HD12	1:L:88:PRO:HD2	1.05	1.04
1:B:296:ARG:HH11	1:B:296:ARG:HG2	1.17	1.03
1:G:155:PHE:CA	1:G:161:GLY:HA3	1.88	1.03
1:J:219:GLU:OE1	1:J:283:GLN:HB2	1.57	1.03
1:D:82:VAL:CG2	1:D:87:LEU:HD22	1.87	1.03
1:J:349:PHE:HB2	1:J:352:SER:HB3	1.34	1.03
1:E:42:ASP:OD1	1:E:565:ARG:NH1	1.91	1.02
1:J:396:VAL:HG23	1:J:404:LEU:HD11	1.40	1.02
1:A:83:VAL:HG21	1:B:17:MET:HE1	1.41	1.02
1:J:354:THR:HG21	1:J:381:TYR:HE2	1.17	1.02
1:E:175:LYS:NZ	1:E:523:GLN:O	1.90	1.02
1:B:42:ASP:OD1	1:B:565:ARG:NH1	1.91	1.02
1:D:103:ASP:HB3	1:D:104:PRO:HD3	1.03	1.02
1:A:42:ASP:OD1	1:A:565:ARG:NH1	1.92	1.01
1:B:277:ILE:HD11	1:B:434:TYR:CD2	1.95	1.01
1:C:42:ASP:OD1	1:C:565:ARG:NH1	1.92	1.01
1:A:349:PHE:CZ	1:A:356:PRO:HB3	1.96	1.01
1:L:376:ILE:HD13	1:L:411:LEU:HB3	1.42	1.01
1:H:42:ASP:OD1	1:H:565:ARG:NH1	1.95	1.00
1:K:192:MET:O	1:K:196:ALA:CB	2.09	1.00
1:K:235:GLU:OE2	1:K:248:ARG:NH1	1.93	1.00
1:J:396:VAL:HG21	1:J:404:LEU:HD11	1.41	1.00
1:D:103:ASP:CB	1:D:104:PRO:HD3	1.92	0.99
1:A:388:GLU:O	1:A:388:GLU:CD	2.05	0.99
1:G:42:ASP:OD1	1:G:565:ARG:NH1	1.95	0.99
1:G:155:PHE:HA	1:G:161:GLY:CA	1.92	0.98
1:D:42:ASP:OD1	1:D:565:ARG:NH1	1.95	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:135:GLU:OE2	1:D:154:ARG:NH2	1.97	0.97
1:G:103:ASP:HB3	1:G:104:PRO:HD3	1.41	0.97
1:K:42:ASP:OD1	1:K:565:ARG:NH1	1.95	0.97
1:K:472:TYR:OH	1:K:476:VAL:HG21	1.64	0.97
1:D:70:HIS:HB3	1:D:73:VAL:HG21	1.44	0.97
1:E:175:LYS:HZ2	1:E:523:GLN:C	1.67	0.96
1:F:42:ASP:OD1	1:F:565:ARG:NH1	1.97	0.96
1:J:174:THR:HG22	3:J:1001:ADP:H5'2	1.47	0.96
1:J:282:ASP:HB3	1:K:202:ARG:NH1	1.78	0.96
1:D:70:HIS:HB3	1:D:73:VAL:CG2	1.95	0.96
1:B:174:THR:HG22	3:B:1001:ADP:H5'2	1.48	0.96
1:B:215:ASN:ND2	1:B:449:ASP:OD1	1.99	0.95
1:D:175:LYS:HG3	3:D:1001:ADP:O1B	1.64	0.95
1:J:598:ARG:O	1:J:601:VAL:HG12	1.68	0.94
1:K:383:LEU:HD22	1:K:396:VAL:HG12	1.48	0.94
1:L:223:PHE:HE1	1:L:284:ARG:HB2	1.32	0.93
1:H:376:ILE:HD13	1:H:411:LEU:HB3	1.50	0.93
1:J:349:PHE:CZ	1:J:356:PRO:HB3	2.03	0.93
1:C:104:PRO:N	1:C:104:PRO:C	2.25	0.93
1:L:14:ALA:HA	1:L:117:ARG:HG2	1.49	0.93
1:L:87:LEU:CD1	1:L:88:PRO:HD2	1.97	0.93
1:G:387:ARG:C	1:G:388:GLU:OE1	2.10	0.92
1:L:86:LEU:H	1:L:86:LEU:HD22	1.30	0.92
1:D:161:GLY:CA	1:D:513:ARG:HE	1.83	0.92
1:K:142:LEU:HD12	1:K:248:ARG:HG2	1.52	0.91
1:L:354:THR:HG1	1:L:355:PRO:HD2	0.83	0.91
1:I:33:VAL:HB	1:I:93:TYR:CD2	2.06	0.91
1:I:219:GLU:HG3	1:I:222:LEU:HD22	1.52	0.91
1:J:396:VAL:HG13	1:J:396:VAL:O	1.68	0.91
1:K:247:ASP:O	1:K:251:LEU:HD12	1.69	0.91
1:A:386:GLU:HB3	1:A:391:GLY:HA2	1.53	0.91
1:I:173:ALA:HB1	1:I:543:GLY:HA3	1.51	0.91
1:E:174:THR:HG22	3:E:1001:ADP:O4'	1.71	0.90
1:K:473:LYS:CG	1:K:517:ILE:CG1	2.48	0.90
1:H:242:LYS:NZ	1:H:588:ASN:ND2	2.20	0.90
1:D:161:GLY:CA	1:D:513:ARG:HH21	1.82	0.90
1:G:387:ARG:O	1:G:388:GLU:CD	2.15	0.90
1:C:57:VAL:HA	1:C:104:PRO:HG2	1.51	0.90
1:L:223:PHE:CE1	1:L:284:ARG:HB2	2.07	0.90
1:J:354:THR:CG2	1:J:381:TYR:CE2	2.56	0.89
1:J:324:ILE:CD1	1:J:407:PHE:CE2	2.54	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:142:LEU:HG	1:K:252:LEU:HD11	1.53	0.89
1:B:295:ILE:HD13	1:B:422:ILE:HG22	1.54	0.89
1:F:597:ARG:NH2	1:F:599:ASP:OD2	2.05	0.89
1:H:223:PHE:CZ	1:H:598:ARG:HD2	2.08	0.88
1:A:174:THR:HG22	3:A:1001:ADP:H5'2	1.54	0.88
1:H:223:PHE:CZ	1:H:598:ARG:CD	2.56	0.88
1:A:155:PHE:HA	1:A:161:GLY:HA3	1.55	0.88
1:B:223:PHE:HA	1:B:284:ARG:NH1	1.87	0.88
1:L:42:ASP:OD1	1:L:565:ARG:NH1	2.07	0.88
1:A:155:PHE:HD2	1:A:579:PRO:HG2	1.38	0.88
1:E:175:LYS:HZ1	1:E:523:GLN:C	1.81	0.88
1:K:174:THR:HB	3:K:1001:ADP:H5'2	1.55	0.88
1:B:268:PRO:CG	1:B:292:VAL:HG12	2.04	0.87
1:K:57:VAL:HA	1:K:104:PRO:HG2	1.57	0.87
1:H:147:GLN:HA	1:H:147:GLN:NE2	1.87	0.87
1:J:405:ARG:O	1:J:409:ARG:N	2.06	0.87
1:F:135:GLU:OE2	1:F:154:ARG:NH2	2.08	0.87
1:K:215:ASN:O	1:K:215:ASN:ND2	2.07	0.87
1:A:473:LYS:NZ	1:A:480:ASP:O	2.08	0.87
1:J:597:ARG:HG3	1:J:599:ASP:OD1	1.73	0.87
1:G:238:VAL:HG11	1:G:248:ARG:HH21	1.40	0.86
1:K:215:ASN:ND2	1:K:218:GLY:O	2.06	0.86
1:B:218:GLY:HA2	1:B:451:HIS:CG	2.11	0.86
1:K:472:TYR:CZ	1:K:476:VAL:HG21	2.10	0.86
1:B:210:ARG:HB2	1:B:482:VAL:HG22	1.55	0.86
1:E:174:THR:CB	3:E:1001:ADP:H5'2	2.05	0.86
1:A:86:LEU:O	1:A:86:LEU:HD22	1.76	0.86
1:B:268:PRO:HG2	1:B:292:VAL:HG12	1.57	0.86
1:L:350:GLU:OE1	1:L:351:ASP:HB2	1.74	0.85
1:E:174:THR:HB	3:E:1001:ADP:H5'2	1.58	0.85
1:I:375:LEU:HD12	1:I:375:LEU:O	1.76	0.85
1:K:174:THR:CB	3:K:1001:ADP:H5'2	2.05	0.85
1:I:142:LEU:CB	1:I:588:ASN:HD21	1.88	0.85
1:K:472:TYR:HE1	1:K:476:VAL:HG11	1.36	0.85
1:C:238:VAL:HG11	1:C:248:ARG:HH21	1.41	0.85
1:K:304:LEU:O	1:K:304:LEU:HD22	1.76	0.85
1:H:223:PHE:HD1	1:H:601:VAL:HG21	1.39	0.85
1:D:352:SER:OG	1:D:385:GLU:OE2	1.95	0.85
1:A:349:PHE:HE1	1:A:356:PRO:HG3	1.42	0.85
1:E:473:LYS:HG3	1:E:517:ILE:HD11	1.57	0.85
1:B:296:ARG:HB2	1:B:340:THR:O	1.76	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:42:ASP:OD1	1:J:565:ARG:NH1	2.09	0.84
1:A:142:LEU:HG	1:A:252:LEU:HD11	1.59	0.84
1:J:198:GLY:O	1:L:597:ARG:NH2	2.09	0.84
1:E:249:TYR:CE1	1:E:590:PRO:HB2	2.12	0.84
1:K:269:ARG:HG3	1:K:269:ARG:O	1.76	0.84
1:C:103:ASP:HB3	1:C:104:PRO:HD3	1.58	0.84
1:J:324:ILE:HD13	1:J:407:PHE:CE2	2.13	0.84
1:L:354:THR:HG1	1:L:355:PRO:CD	1.77	0.83
1:D:136:ALA:HB2	1:D:154:ARG:HE	1.43	0.83
1:J:349:PHE:HZ	1:J:356:PRO:HB3	1.42	0.83
1:K:246:ALA:O	1:K:251:LEU:HD11	1.78	0.83
1:D:396:VAL:HG23	1:D:404:LEU:HD11	1.59	0.83
1:I:87:LEU:HD12	1:I:88:PRO:HD2	0.83	0.83
1:L:357:GLU:OE2	1:L:358:ASN:OD1	1.95	0.83
1:E:248:ARG:HH11	1:E:590:PRO:HA	1.41	0.83
1:B:331:LEU:HD23	1:B:342:LEU:HD21	1.60	0.82
1:L:218:GLY:HA2	1:L:451:HIS:CD2	2.14	0.82
1:A:230:ARG:NH1	1:A:599:ASP:OD1	2.12	0.82
1:C:135:GLU:OE2	1:C:154:ARG:NH2	2.13	0.82
1:J:455:ALA:HB2	1:K:511:ARG:CD	2.09	0.82
1:G:135:GLU:OE2	1:G:154:ARG:NH2	2.12	0.82
1:F:238:VAL:HG11	1:F:248:ARG:HH21	1.45	0.82
1:J:401:PRO:HB2	1:K:397:LEU:HB3	1.61	0.82
1:A:349:PHE:CE1	1:A:356:PRO:HG3	2.15	0.82
1:B:490:ASN:OD1	1:B:491:LYS:N	2.13	0.81
1:J:215:ASN:HD21	1:J:219:GLU:H	1.27	0.81
1:C:230:ARG:NH1	1:C:599:ASP:OD1	2.12	0.81
1:I:142:LEU:HG	1:I:252:LEU:HD11	1.62	0.81
1:J:378:TYR:OH	1:J:382:LYS:NZ	2.12	0.81
1:H:238:VAL:HG11	1:H:248:ARG:HH21	1.45	0.81
1:J:17:MET:HE1	1:L:83:VAL:HG11	1.63	0.81
1:J:349:PHE:CB	1:J:352:SER:HB3	2.11	0.81
1:E:213:ILE:HG13	1:E:485:VAL:HB	1.61	0.81
1:H:319:PHE:HZ	1:G:315:LEU:HD21	1.46	0.81
1:E:175:LYS:HZ1	1:E:524:GLN:N	1.79	0.81
1:F:566:ALA:HA	1:F:569:LEU:HG	1.62	0.81
1:G:173:ALA:O	3:G:1001:ADP:O3B	1.97	0.81
1:E:176:THR:OG1	3:E:1001:ADP:O3B	1.99	0.81
1:J:402:GLY:C	1:K:319:PHE:CE1	2.58	0.81
1:E:149:LEU:HD12	1:E:150:PRO:HD2	1.62	0.81
1:E:175:LYS:NZ	1:E:524:GLN:N	2.28	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:238:VAL:HG11	1:J:248:ARG:HH21	1.46	0.81
1:K:315:LEU:HB3	1:K:317:LEU:HD13	1.60	0.80
1:J:566:ALA:HA	1:J:569:LEU:HG	1.63	0.80
1:K:247:ASP:O	1:K:251:LEU:CD1	2.29	0.80
1:C:208:GLY:O	1:C:480:ASP:HB2	1.81	0.80
1:E:249:TYR:CE1	1:E:590:PRO:CB	2.64	0.80
1:I:101:ARG:NH2	1:I:131:ASP:OD2	2.14	0.80
1:C:210:ARG:NH1	1:C:443:ILE:O	2.14	0.80
1:J:282:ASP:CB	1:K:202:ARG:NH1	2.41	0.80
1:B:296:ARG:HG2	1:B:296:ARG:NH1	1.91	0.80
1:J:402:GLY:HA3	1:K:319:PHE:CD1	2.17	0.80
1:J:324:ILE:HD12	1:J:407:PHE:CZ	2.16	0.80
1:A:57:VAL:HA	1:A:104:PRO:HG2	1.64	0.80
1:F:282:ASP:N	1:F:282:ASP:OD1	2.09	0.80
1:K:215:ASN:ND2	1:K:451:HIS:HD2	1.80	0.80
1:K:472:TYR:CE1	1:K:476:VAL:CG1	2.64	0.80
1:K:513:ARG:HH11	1:K:513:ARG:HB2	1.48	0.79
1:A:320:VAL:HG22	1:A:399:GLN:HG2	1.62	0.79
1:F:386:GLU:HB3	1:F:391:GLY:HA2	1.65	0.79
1:J:402:GLY:C	1:K:319:PHE:CD1	2.61	0.79
1:G:109:PRO:HG3	1:I:66:VAL:HG13	1.64	0.79
1:K:213:ILE:HD13	1:K:221:LEU:CD2	2.12	0.79
1:K:597:ARG:CG	1:K:600:GLU:HG3	2.12	0.79
1:D:162:GLY:HA3	1:D:538:ALA:CB	2.13	0.79
1:L:238:VAL:HG11	1:L:248:ARG:HH21	1.47	0.79
1:K:383:LEU:HD23	1:K:396:VAL:HG13	1.65	0.79
1:I:423:ARG:HG2	1:I:423:ARG:HH11	1.48	0.78
1:G:386:GLU:HB3	1:G:391:GLY:HA2	1.63	0.78
1:B:396:VAL:CG2	1:B:404:LEU:HD11	2.11	0.78
1:K:383:LEU:CD2	1:K:396:VAL:HG12	2.12	0.78
1:D:201:GLY:HA2	1:D:204:SER:OG	1.83	0.78
1:K:155:PHE:HA	1:K:161:GLY:HA3	1.66	0.78
1:C:400:SER:HB2	1:D:398:LYS:NZ	1.99	0.78
1:D:161:GLY:HA2	1:D:513:ARG:HE	1.46	0.78
1:B:223:PHE:CE1	1:B:284:ARG:HB2	2.19	0.77
1:I:405:ARG:HH21	1:I:405:ARG:HG3	1.49	0.77
1:K:213:ILE:HG13	1:K:485:VAL:HB	1.65	0.77
1:J:396:VAL:O	1:J:396:VAL:CG1	2.33	0.77
1:K:57:VAL:HG13	1:K:104:PRO:HD2	1.67	0.77
1:H:242:LYS:NZ	1:H:588:ASN:HD21	1.82	0.77
1:J:324:ILE:CD1	1:J:407:PHE:CZ	2.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:230:ARG:NH1	1:H:599:ASP:OD1	2.17	0.77
1:K:473:LYS:CG	1:K:517:ILE:HG13	2.14	0.77
1:H:412:ARG:HH11	1:H:415:GLN:HE22	1.33	0.77
1:L:26:PRO:HD3	1:L:109:PRO:HG3	1.64	0.77
1:C:202:ARG:NH2	1:C:202:ARG:HG3	2.00	0.77
1:E:175:LYS:HZ3	1:E:524:GLN:HA	1.48	0.77
1:K:304:LEU:HD13	1:K:321:ILE:HG23	1.67	0.76
1:C:202:ARG:HG3	1:C:202:ARG:HH21	1.49	0.76
1:K:473:LYS:HD2	1:K:515:LEU:O	1.84	0.76
1:A:76:GLU:HA	1:B:21:THR:HG21	1.67	0.76
1:B:478:ARG:HG3	1:B:516:GLY:HA3	1.66	0.76
1:I:33:VAL:CB	1:I:93:TYR:CD2	2.68	0.76
1:L:49:THR:OG1	1:L:114:ASP:OD2	2.04	0.76
1:A:197:GLN:OE1	1:A:197:GLN:HA	1.84	0.76
1:A:248:ARG:NH1	1:A:589:TYR:O	2.19	0.76
1:L:349:PHE:HB2	1:L:352:SER:HB3	1.65	0.76
1:K:136:ALA:HA	1:K:195:THR:CG2	2.15	0.76
1:D:354:THR:OG1	1:D:355:PRO:HD2	1.85	0.76
1:K:135:GLU:OE2	1:K:154:ARG:NH2	2.17	0.76
1:B:387:ARG:HB2	1:B:390:GLU:HG2	1.68	0.76
1:D:162:GLY:HA3	1:D:538:ALA:HB2	1.68	0.76
1:K:286:GLU:HG2	1:K:286:GLU:O	1.85	0.76
1:I:33:VAL:HB	1:I:93:TYR:HD2	1.47	0.75
1:K:173:ALA:HB1	1:K:543:GLY:HA3	1.67	0.75
1:K:296:ARG:NH1	1:K:339:GLY:O	2.19	0.75
1:K:513:ARG:HB2	1:K:513:ARG:NH1	2.00	0.75
1:E:210:ARG:NH1	1:E:443:ILE:O	2.19	0.75
1:K:355:PRO:HB2	1:K:357:GLU:HG3	1.68	0.75
1:K:449:ASP:OD1	1:K:451:HIS:CD2	2.39	0.75
1:C:315:LEU:HD22	1:D:319:PHE:HZ	1.50	0.75
1:I:397:LEU:HB3	1:K:401:PRO:HG2	1.67	0.75
1:A:155:PHE:CE2	1:A:579:PRO:HG2	2.21	0.75
1:B:219:GLU:CA	1:B:222:LEU:CD1	2.64	0.75
1:D:350:GLU:HG2	1:D:351:ASP:N	2.01	0.75
1:G:230:ARG:NH1	1:G:599:ASP:OD1	2.20	0.75
1:L:218:GLY:H	1:L:451:HIS:HB2	1.50	0.75
1:D:566:ALA:HA	1:D:569:LEU:HG	1.67	0.75
1:K:597:ARG:HG3	1:K:600:GLU:HG3	1.69	0.74
1:L:86:LEU:HD22	1:L:86:LEU:N	2.02	0.74
1:E:174:THR:CG2	3:E:1001:ADP:O4'	2.34	0.74
1:J:402:GLY:CA	1:K:319:PHE:CD1	2.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:70:HIS:CB	1:D:73:VAL:HG21	2.18	0.74
1:F:165:ASN:HD21	1:F:523:GLN:HE22	1.33	0.74
1:B:282:ASP:OD2	1:C:202:ARG:HD3	1.88	0.74
1:E:101:ARG:HH12	1:E:132:LYS:HE2	1.52	0.74
1:I:588:ASN:HD22	1:I:588:ASN:H	1.36	0.74
1:H:315:LEU:HD22	1:L:319:PHE:HZ	1.52	0.74
1:L:154:ARG:NH1	1:L:159:GLU:OE2	2.20	0.74
1:J:87:LEU:O	1:J:87:LEU:HD22	1.88	0.74
1:L:215:ASN:HB3	1:L:449:ASP:HA	1.69	0.74
1:E:149:LEU:HD21	1:E:576:VAL:HG21	1.67	0.74
1:E:225:ASP:OD1	1:E:226:LYS:N	2.21	0.74
1:K:384:LEU:HD22	1:K:405:ARG:HH11	1.52	0.73
1:H:320:VAL:HG22	1:H:399:GLN:HG2	1.68	0.73
1:D:76:GLU:HB3	1:E:71:GLU:OE2	1.87	0.73
1:I:23:ASP:OD1	1:K:69:ARG:NE	2.21	0.73
1:I:135:GLU:OE2	1:I:154:ARG:NH2	2.19	0.73
1:L:597:ARG:NH2	1:L:599:ASP:OD2	2.22	0.73
1:H:149:LEU:HD23	1:H:587:VAL:HG11	1.70	0.73
1:A:146:GLY:HA2	1:A:251:LEU:HD23	1.70	0.73
1:I:376:ILE:HD13	1:I:411:LEU:HB3	1.70	0.73
1:J:103:ASP:HB3	1:J:104:PRO:HD3	1.71	0.73
1:H:549:GLU:OE2	1:L:531:ARG:NH2	2.22	0.73
1:A:388:GLU:O	1:A:388:GLU:OE1	2.05	0.73
1:I:397:LEU:HD22	1:I:397:LEU:N	2.03	0.73
1:C:386:GLU:HB3	1:C:391:GLY:HA2	1.71	0.73
1:F:173:ALA:O	3:F:1001:ADP:O1B	2.06	0.73
1:E:219:GLU:OE1	1:E:283:GLN:HB2	1.88	0.73
1:I:511:ARG:NH1	1:K:456:HIS:HE1	1.86	0.73
1:L:133:MET:SD	1:L:150:PRO:HB2	2.28	0.73
1:A:349:PHE:HZ	1:A:356:PRO:HB3	1.50	0.73
1:K:383:LEU:CD2	1:K:396:VAL:CG1	2.66	0.73
1:L:86:LEU:H	1:L:86:LEU:CD2	2.01	0.73
1:H:135:GLU:OE2	1:H:154:ARG:NH2	2.20	0.73
1:G:263:GLN:HE21	1:G:265:LEU:HD21	1.54	0.72
1:K:309:SER:HB2	1:K:500:PRO:HD2	1.71	0.72
1:C:400:SER:HB2	1:D:398:LYS:HZ3	1.54	0.72
1:G:323:ASN:OD1	1:I:405:ARG:HD2	1.89	0.72
1:J:402:GLY:CA	1:K:319:PHE:HD1	2.01	0.72
1:C:396:VAL:HG23	1:C:404:LEU:HD11	1.70	0.72
1:D:87:LEU:HD23	1:D:87:LEU:C	2.13	0.72
1:L:215:ASN:ND2	1:L:449:ASP:OD1	2.21	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:231:MET:HE1	1:L:256:ALA:HB1	1.72	0.72
1:H:19:LEU:HD13	1:H:32:ALA:HB2	1.72	0.72
1:H:219:GLU:CD	1:H:283:GLN:HB2	2.14	0.72
1:H:412:ARG:HH11	1:H:415:GLN:NE2	1.87	0.72
1:A:149:LEU:HD21	1:A:576:VAL:HG21	1.70	0.72
1:B:218:GLY:CA	1:B:451:HIS:CD2	2.72	0.72
1:J:310:ASP:OD2	1:J:314:SER:HB3	1.90	0.72
1:J:359:LEU:HD22	1:J:374:GLN:NE2	2.04	0.72
1:A:149:LEU:HD22	1:A:587:VAL:HG11	1.70	0.72
1:B:219:GLU:HA	1:B:222:LEU:HD12	1.72	0.72
1:K:304:LEU:HD22	1:K:304:LEU:C	2.14	0.72
1:K:473:LYS:HG3	1:K:517:ILE:HG13	1.72	0.72
1:J:135:GLU:OE2	1:J:154:ARG:NH2	2.21	0.71
1:E:320:VAL:HG22	1:E:399:GLN:HG2	1.72	0.71
1:B:349:PHE:HB2	1:B:352:SER:HB3	1.72	0.71
1:L:248:ARG:NH1	1:L:589:TYR:O	2.23	0.71
1:I:228:ASN:ND2	1:I:600:GLU:HB3	2.05	0.71
1:I:29:PHE:CZ	1:I:47:VAL:HG11	2.26	0.71
1:I:338:LYS:HE3	1:I:428:PRO:HG2	1.73	0.71
1:K:310:ASP:OD2	1:K:456:HIS:CG	2.43	0.71
1:E:386:GLU:HB3	1:E:391:GLY:HA2	1.71	0.71
1:L:163:HIS:HB2	1:L:537:ALA:HA	1.73	0.71
1:C:208:GLY:O	1:C:480:ASP:CB	2.39	0.71
1:E:173:ALA:HB1	1:E:543:GLY:HA3	1.73	0.71
1:F:248:ARG:NH1	1:F:589:TYR:O	2.24	0.71
3:A:1001:ADP:O1A	3:A:1001:ADP:H3'	1.90	0.71
1:C:155:PHE:CA	1:C:161:GLY:HA3	2.18	0.71
1:I:566:ALA:HA	1:I:569:LEU:HG	1.72	0.70
1:A:143:LEU:HD12	1:A:143:LEU:C	2.15	0.70
1:J:21:THR:HG23	1:L:79:VAL:HG21	1.72	0.70
1:H:149:LEU:HD12	1:H:150:PRO:HD2	1.73	0.70
1:B:218:GLY:HA3	1:B:451:HIS:CD2	2.26	0.70
1:J:406:ALA:HA	1:J:409:ARG:HG2	1.74	0.70
1:C:231:MET:HE1	1:C:256:ALA:CB	2.17	0.70
1:K:174:THR:CG2	3:K:1001:ADP:H5'2	2.21	0.70
1:L:192:MET:O	1:L:196:ALA:HB2	1.92	0.70
1:L:291:PHE:HB2	1:L:436:PRO:HG3	1.74	0.70
1:K:396:VAL:HG23	1:K:396:VAL:O	1.91	0.70
1:A:291:PHE:HB2	1:A:436:PRO:HG3	1.74	0.70
1:D:263:GLN:HB2	1:D:443:ILE:HG21	1.74	0.70
1:B:248:ARG:NH1	1:B:589:TYR:O	2.25	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:405:ARG:HG3	1:I:405:ARG:NH2	2.06	0.70
1:K:304:LEU:CD1	1:K:321:ILE:HG23	2.21	0.70
1:B:75:PHE:CD1	1:C:71:GLU:HG3	2.27	0.70
1:B:174:THR:CG2	3:B:1001:ADP:H5'2	2.20	0.70
1:I:373:GLU:OE1	1:I:373:GLU:N	2.24	0.70
1:K:368:ASN:HD22	1:K:370:GLN:HG2	1.56	0.70
1:A:238:VAL:HG11	1:A:248:ARG:HH21	1.55	0.69
1:B:103:ASP:HB3	1:B:104:PRO:HD3	1.72	0.69
1:G:309:SER:O	1:G:309:SER:OG	2.04	0.69
1:C:315:LEU:HG	1:C:316:ASN:N	2.07	0.69
1:I:71:GLU:OE1	1:K:76:GLU:HB3	1.93	0.69
1:K:142:LEU:HG	1:K:252:LEU:CD1	2.22	0.69
1:A:103:ASP:HB3	1:A:104:PRO:HD3	1.74	0.69
1:B:470:PHE:CE1	1:B:515:LEU:HD23	2.27	0.69
1:D:136:ALA:HB2	1:D:154:ARG:NE	2.06	0.69
1:G:597:ARG:HG2	1:G:600:GLU:HG3	1.75	0.69
1:I:353:GLU:OE1	1:I:353:GLU:HA	1.91	0.69
3:J:1001:ADP:O1A	3:J:1001:ADP:H3'	1.92	0.69
1:I:261:ASP:HB2	1:I:444:GLN:H	1.55	0.69
1:A:174:THR:CG2	3:A:1001:ADP:H5'2	2.22	0.69
1:F:598:ARG:O	1:F:601:VAL:HG12	1.91	0.69
1:I:511:ARG:HH12	1:K:456:HIS:HE1	1.37	0.69
1:C:383:LEU:HG	1:C:404:LEU:HD13	1.74	0.69
1:D:58:ARG:HB2	1:D:103:ASP:HB2	1.74	0.69
1:K:310:ASP:OD2	1:K:456:HIS:CD2	2.46	0.69
1:L:566:ALA:HA	1:L:569:LEU:HG	1.75	0.69
1:C:19:LEU:HD13	1:C:32:ALA:HB2	1.73	0.69
1:D:19:LEU:HD13	1:D:32:ALA:HB2	1.75	0.69
1:F:142:LEU:HG	1:F:252:LEU:HD11	1.73	0.69
1:J:87:LEU:HD13	1:J:87:LEU:H	1.56	0.69
1:K:530:GLU:OE2	1:K:532:ARG:HD3	1.93	0.69
1:D:392:ASP:O	1:D:396:VAL:HG12	1.93	0.69
1:J:579:PRO:O	1:L:544:ARG:NH1	2.26	0.69
1:K:383:LEU:HD23	1:K:396:VAL:CG1	2.21	0.69
1:H:218:GLY:HA2	1:H:451:HIS:HB2	1.75	0.68
1:I:356:PRO:HA	1:I:359:LEU:HD22	1.75	0.68
1:K:103:ASP:HB3	1:K:104:PRO:HD3	1.74	0.68
1:H:223:PHE:CZ	1:H:598:ARG:HD3	2.27	0.68
1:A:153:PHE:CE2	1:A:195:THR:HG21	2.27	0.68
1:B:373:GLU:OE1	1:B:373:GLU:N	2.23	0.68
1:D:350:GLU:HG2	1:D:351:ASP:H	1.57	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:247:ASP:OD1	1:K:247:ASP:N	2.24	0.68
1:K:350:GLU:OE1	1:K:350:GLU:HA	1.93	0.68
1:D:161:GLY:CA	1:D:513:ARG:NH2	2.55	0.68
1:E:143:LEU:C	1:E:143:LEU:HD12	2.18	0.68
1:A:83:VAL:HG21	1:B:17:MET:CE	2.22	0.68
1:B:297:GLU:HA	1:B:297:GLU:OE2	1.92	0.68
1:B:383:LEU:HD22	1:B:404:LEU:HD22	1.76	0.68
1:J:218:GLY:HA2	1:J:451:HIS:CB	2.23	0.68
1:K:246:ALA:C	1:K:251:LEU:HD11	2.19	0.68
1:E:228:ASN:ND2	1:E:600:GLU:OE1	2.21	0.68
1:I:155:PHE:HA	1:I:161:GLY:HA3	1.73	0.68
1:L:60:TYR:HE1	1:L:103:ASP:HB2	1.57	0.68
1:L:149:LEU:HD22	1:L:587:VAL:HG11	1.76	0.68
1:B:135:GLU:OE2	1:B:154:ARG:NH2	2.27	0.68
1:B:293:PHE:O	1:B:422:ILE:HA	1.92	0.68
1:D:348:GLN:OE1	1:J:348:GLN:NE2	2.21	0.68
1:E:19:LEU:HD13	1:E:32:ALA:HB2	1.75	0.68
1:B:267:PRO:HD3	1:B:449:ASP:O	1.94	0.68
1:C:142:LEU:HG	1:C:252:LEU:HD11	1.74	0.68
1:C:149:LEU:HD13	1:C:585:VAL:HG21	1.75	0.68
1:I:375:LEU:HD12	1:I:375:LEU:C	2.16	0.68
1:A:149:LEU:HD13	1:A:585:VAL:HG21	1.76	0.68
1:L:84:ALA:HB3	1:L:86:LEU:CD2	2.24	0.68
1:L:102:VAL:HG23	1:L:105:GLU:HA	1.76	0.68
1:L:349:PHE:HB2	1:L:352:SER:CB	2.24	0.68
1:B:180:LEU:HD11	1:B:221:LEU:HD21	1.74	0.67
1:B:597:ARG:NH2	1:B:599:ASP:OD2	2.27	0.67
1:F:263:GLN:HE21	1:F:265:LEU:HD21	1.57	0.67
1:H:354:THR:HG23	1:H:355:PRO:HD2	1.75	0.67
1:L:78:ASP:O	1:L:82:VAL:HG23	1.93	0.67
1:I:399:GLN:OE1	1:I:399:GLN:HA	1.94	0.67
1:K:280:GLN:HG2	1:K:452:ALA:CB	2.25	0.67
1:C:22:GLU:OE2	1:C:67:ARG:NH2	2.25	0.67
1:I:142:LEU:HG	1:I:252:LEU:CD1	2.24	0.67
1:H:358:ASN:OD1	1:H:358:ASN:N	2.27	0.67
1:D:161:GLY:CA	1:D:513:ARG:NE	2.57	0.67
1:A:76:GLU:HB3	1:B:71:GLU:OE2	1.94	0.67
1:B:277:ILE:HD11	1:B:434:TYR:CE2	2.30	0.67
1:J:380:GLU:OE2	1:J:412:ARG:NH2	2.21	0.67
1:L:19:LEU:HD13	1:L:32:ALA:HB2	1.76	0.67
1:C:41:LEU:HB2	1:D:107:PHE:HB3	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:597:ARG:CG	1:C:600:GLU:HG3	2.24	0.67
1:G:279:PRO:HB2	1:G:281:THR:HG23	1.76	0.67
1:I:142:LEU:C	1:I:588:ASN:ND2	2.52	0.66
1:K:228:ASN:ND2	1:K:600:GLU:OE1	2.28	0.66
1:H:223:PHE:HZ	1:H:598:ARG:CD	2.05	0.66
1:I:386:GLU:HB3	1:I:391:GLY:HA2	1.76	0.66
1:I:423:ARG:HG2	1:I:423:ARG:NH1	2.08	0.66
1:J:548:ALA:HB2	1:K:556:ARG:HB2	1.77	0.66
1:A:87:LEU:C	1:A:87:LEU:HD23	2.21	0.66
1:A:347:TRP:CZ2	1:A:354:THR:HG21	2.30	0.66
1:I:495:ARG:NH2	1:I:554:GLU:OE2	2.28	0.66
1:K:163:HIS:HB3	1:K:519:LEU:O	1.94	0.66
1:L:362:SER:N	1:L:366:GLY:O	2.27	0.66
1:L:373:GLU:N	1:L:373:GLU:OE1	2.27	0.66
1:H:388:GLU:HG3	1:E:388:GLU:HG2	1.75	0.66
1:E:149:LEU:CD2	1:E:587:VAL:HG11	2.25	0.66
1:E:184:HIS:CE1	1:E:188:ARG:HG3	2.30	0.66
1:J:349:PHE:O	1:J:349:PHE:CD1	2.47	0.66
1:A:142:LEU:HG	1:A:252:LEU:CD1	2.26	0.66
1:J:401:PRO:CB	1:K:397:LEU:HB3	2.26	0.66
1:I:41:LEU:O	1:I:63:VAL:O	2.14	0.66
1:I:142:LEU:CB	1:I:588:ASN:ND2	2.59	0.66
1:I:215:ASN:HB2	1:I:221:LEU:HB2	1.77	0.66
1:J:215:ASN:HB2	1:J:221:LEU:HB2	1.76	0.66
1:A:155:PHE:HA	1:A:161:GLY:CA	2.24	0.66
1:E:469:VAL:O	1:E:473:LYS:HG2	1.96	0.66
1:G:238:VAL:HG11	1:G:248:ARG:NH2	2.10	0.66
1:K:248:ARG:HA	1:K:251:LEU:HD13	1.78	0.66
1:C:248:ARG:NH1	1:C:589:TYR:O	2.29	0.66
1:H:267:PRO:HB3	1:H:421:LEU:HD21	1.77	0.65
1:B:277:ILE:HD11	1:B:434:TYR:HD2	1.60	0.65
1:C:155:PHE:HA	1:C:161:GLY:CA	2.20	0.65
1:B:478:ARG:O	1:B:478:ARG:HG2	1.96	0.65
1:B:495:ARG:NH2	1:B:554:GLU:OE2	2.29	0.65
1:E:175:LYS:HZ3	1:E:524:GLN:CA	2.10	0.65
1:K:235:GLU:CD	1:K:248:ARG:HH11	2.04	0.65
1:A:153:PHE:CD2	1:A:195:THR:HG21	2.32	0.65
1:E:175:LYS:HD2	1:E:522:ALA:HB1	1.77	0.65
1:B:218:GLY:HA2	1:B:451:HIS:CD2	2.31	0.65
1:K:189:SER:OG	1:K:191:VAL:HG12	1.95	0.65
1:H:412:ARG:NH1	1:H:415:GLN:HE22	1.92	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:MET:HE1	1:F:83:VAL:HG11	1.78	0.65
1:I:142:LEU:HB3	1:I:588:ASN:HD21	1.60	0.65
1:J:398:LYS:HG3	1:J:398:LYS:O	1.96	0.65
1:J:553:PRO:HA	1:J:556:ARG:HD3	1.77	0.65
1:K:188:ARG:HH11	1:K:188:ARG:HG2	1.61	0.65
1:L:103:ASP:HB3	1:L:104:PRO:HD3	1.77	0.65
1:C:242:LYS:HB2	1:C:244:LEU:HD13	1.79	0.65
1:H:195:THR:O	1:H:203:GLN:NE2	2.29	0.65
1:K:299:CYS:HB3	1:K:328:LEU:HB3	1.78	0.65
1:A:553:PRO:O	1:A:556:ARG:HG2	1.97	0.65
1:I:149:LEU:HD22	1:I:587:VAL:HG11	1.77	0.65
1:J:396:VAL:HG21	1:J:404:LEU:CD1	2.24	0.65
1:K:387:ARG:O	1:K:388:GLU:HG2	1.97	0.65
1:A:164:ILE:HG12	1:A:539:ILE:HB	1.79	0.64
1:B:268:PRO:HG3	1:B:292:VAL:HG12	1.76	0.64
1:I:588:ASN:HD22	1:I:588:ASN:N	1.90	0.64
1:H:57:VAL:HA	1:H:104:PRO:HG2	1.77	0.64
1:B:368:ASN:HD22	1:B:370:GLN:HG2	1.61	0.64
1:I:473:LYS:HG3	1:I:517:ILE:HD11	1.78	0.64
1:J:553:PRO:O	1:J:556:ARG:HG2	1.97	0.64
3:K:1001:ADP:H3'	3:K:1001:ADP:O1A	1.96	0.64
1:C:315:LEU:HG	1:C:316:ASN:H	1.63	0.64
1:D:161:GLY:HA2	1:D:513:ARG:NE	2.12	0.64
1:K:215:ASN:ND2	1:K:451:HIS:CD2	2.63	0.64
1:H:473:LYS:NZ	1:H:480:ASP:O	2.28	0.64
1:A:474:GLU:OE1	1:A:511:ARG:NH2	2.29	0.64
1:C:165:ASN:HD21	1:C:523:GLN:HE22	1.43	0.64
1:G:248:ARG:NH1	1:G:589:TYR:O	2.31	0.64
1:D:158:GLY:HA2	1:D:161:GLY:HA2	1.78	0.64
1:I:33:VAL:HG11	1:I:93:TYR:CE2	2.33	0.64
1:I:142:LEU:HB2	1:I:588:ASN:ND2	2.12	0.64
1:L:173:ALA:O	3:L:1001:ADP:O3B	2.16	0.64
1:A:149:LEU:HD21	1:A:576:VAL:CG2	2.27	0.64
1:A:175:LYS:N	3:A:1001:ADP:O1B	2.31	0.64
1:C:566:ALA:HA	1:C:569:LEU:HG	1.80	0.64
1:J:213:ILE:HG12	1:J:221:LEU:CD1	2.27	0.64
1:A:530:GLU:OE2	1:A:532:ARG:HD3	1.97	0.64
1:D:70:HIS:HB3	1:D:73:VAL:HG23	1.76	0.64
1:E:204:SER:O	1:E:479:GLN:O	2.15	0.64
1:K:495:ARG:HH21	1:K:527:SER:HA	1.63	0.64
1:J:359:LEU:CD2	1:J:374:GLN:NE2	2.61	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:597:ARG:HG2	1:K:600:GLU:HG3	1.80	0.64
1:A:566:ALA:HA	1:A:569:LEU:HG	1.79	0.63
1:B:219:GLU:CA	1:B:222:LEU:HD12	2.28	0.63
1:I:103:ASP:HB3	1:I:104:PRO:HD3	1.80	0.63
1:D:324:ILE:HD11	1:D:383:LEU:HD11	1.80	0.63
1:I:400:SER:OG	1:I:401:PRO:HD2	1.98	0.63
1:I:421:LEU:HD11	1:I:453:LEU:HD13	1.81	0.63
1:J:86:LEU:HD23	1:J:86:LEU:N	2.12	0.63
1:D:201:GLY:CA	1:D:204:SER:OG	2.46	0.63
1:J:354:THR:CG2	1:J:381:TYR:CZ	2.81	0.63
1:G:566:ALA:HA	1:G:569:LEU:HG	1.81	0.63
1:J:402:GLY:C	1:K:319:PHE:HE1	2.06	0.63
1:J:405:ARG:NE	1:K:323:ASN:OD1	2.32	0.63
1:H:91:VAL:HG11	1:L:111:GLN:HE22	1.64	0.63
1:G:315:LEU:HB3	1:G:317:LEU:HD13	1.81	0.63
1:I:547:LEU:HD12	1:I:547:LEU:H	1.63	0.63
1:L:19:LEU:H	1:L:31:PHE:HA	1.62	0.63
1:L:222:LEU:N	1:L:222:LEU:HD12	2.13	0.63
1:H:218:GLY:HA2	1:H:451:HIS:CB	2.29	0.63
1:D:161:GLY:HA3	1:D:513:ARG:HH21	1.63	0.63
1:B:189:SER:O	1:B:194:ARG:NH2	2.32	0.63
1:F:335:GLN:NE2	1:F:343:ILE:O	2.31	0.63
1:I:51:LYS:NZ	1:I:106:ASN:ND2	2.47	0.63
1:D:82:VAL:HG22	1:D:87:LEU:CD2	2.16	0.63
1:E:566:ALA:HA	1:E:569:LEU:HD13	1.80	0.63
1:G:19:LEU:HD13	1:G:32:ALA:HB2	1.81	0.63
1:G:547:LEU:H	1:G:547:LEU:HD12	1.64	0.63
1:J:291:PHE:HB2	1:J:436:PRO:HG3	1.78	0.63
1:B:19:LEU:HD13	1:B:32:ALA:HB2	1.81	0.62
1:E:453:LEU:HB3	1:E:457:ALA:HB3	1.80	0.62
1:J:346:ASP:OD2	1:J:382:LYS:NZ	2.23	0.62
1:H:547:LEU:HD22	1:L:557:PHE:HA	1.80	0.62
1:C:597:ARG:HG2	1:C:600:GLU:HG3	1.81	0.62
1:F:189:SER:O	1:F:194:ARG:NH2	2.32	0.62
1:J:60:TYR:HE2	1:J:103:ASP:HB2	1.64	0.62
1:H:196:ALA:HA	1:H:203:GLN:NE2	2.14	0.62
1:E:473:LYS:HG3	1:E:517:ILE:CD1	2.26	0.62
1:F:269:ARG:HA	1:F:280:GLN:HG2	1.82	0.62
1:F:396:VAL:HG13	1:F:404:LEU:HD11	1.79	0.62
1:K:247:ASP:C	1:K:251:LEU:CD1	2.72	0.62
1:B:530:GLU:HG3	1:B:532:ARG:H	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:203:GLN:OE1	1:D:203:GLN:HA	1.99	0.62
1:F:156:ILE:O	1:F:162:GLY:O	2.18	0.62
1:I:51:LYS:NZ	1:I:106:ASN:HD21	1.97	0.62
1:E:76:GLU:HG2	1:F:71:GLU:OE2	1.99	0.62
1:B:474:GLU:OE1	1:B:511:ARG:NH2	2.32	0.62
1:E:227:PRO:HA	1:E:258:PRO:HG3	1.81	0.62
1:G:387:ARG:C	1:G:388:GLU:CD	2.64	0.62
1:I:219:GLU:O	1:I:219:GLU:HG2	1.99	0.62
1:J:335:GLN:NE2	1:J:343:ILE:O	2.31	0.62
1:E:149:LEU:HD12	1:E:150:PRO:CD	2.30	0.62
1:I:60:TYR:O	1:I:99:VAL:HG13	1.98	0.62
1:A:24:VAL:HG12	1:A:110:PRO:HD2	1.80	0.62
1:D:320:VAL:HG22	1:D:399:GLN:HG2	1.81	0.62
1:K:162:GLY:H	1:K:538:ALA:HB2	1.65	0.62
1:B:165:ASN:HD21	1:B:523:GLN:HE22	1.48	0.62
1:C:393:PRO:O	1:C:397:LEU:HD23	1.98	0.62
1:G:202:ARG:NH1	1:G:202:ARG:HB3	2.15	0.62
1:K:136:ALA:HA	1:K:195:THR:HG22	1.80	0.62
1:G:166:ILE:HG22	1:G:175:LYS:HB3	1.80	0.62
1:J:20:GLY:HA3	1:L:70:HIS:HB2	1.82	0.62
1:J:76:GLU:HA	1:K:21:THR:HG21	1.81	0.62
1:J:174:THR:CG2	3:J:1001:ADP:H5'2	2.28	0.62
1:K:277:ILE:O	1:K:277:ILE:HG22	1.99	0.62
1:K:73:VAL:HG23	1:K:73:VAL:O	2.00	0.61
1:A:155:PHE:CE2	1:A:579:PRO:HB2	2.35	0.61
1:B:230:ARG:NH1	1:B:599:ASP:OD1	2.32	0.61
1:B:488:GLU:HB3	1:B:491:LYS:HG2	1.82	0.61
1:E:225:ASP:OD1	1:E:226:LYS:HG2	2.00	0.61
1:F:405:ARG:HA	1:F:408:THR:HB	1.82	0.61
1:K:184:HIS:ND1	1:K:594:TRP:HZ3	1.97	0.61
1:H:388:GLU:CG	1:E:388:GLU:HG2	2.30	0.61
1:D:354:THR:OG1	1:D:355:PRO:CD	2.47	0.61
1:E:165:ASN:OD1	1:E:523:GLN:NE2	2.28	0.61
1:E:173:ALA:HB2	1:E:544:ARG:H	1.65	0.61
1:I:173:ALA:CB	1:I:543:GLY:HA3	2.28	0.61
1:I:222:LEU:N	1:I:222:LEU:HD12	2.15	0.61
1:A:86:LEU:HD22	1:A:86:LEU:C	2.23	0.61
1:F:195:THR:HG23	1:F:203:GLN:HE22	1.65	0.61
1:J:396:VAL:HG23	1:J:404:LEU:CD1	2.26	0.61
1:K:219:GLU:OE1	1:K:283:GLN:CD	2.43	0.61
1:K:219:GLU:OE1	1:K:283:GLN:NE2	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:357:GLU:O	1:L:359:LEU:HD13	1.99	0.61
1:E:473:LYS:CG	1:E:517:ILE:HD11	2.27	0.61
1:I:291:PHE:HB2	1:I:436:PRO:HG3	1.83	0.61
1:K:472:TYR:CZ	1:K:476:VAL:CG2	2.83	0.61
1:H:19:LEU:HD11	1:G:76:GLU:HB2	1.82	0.61
1:A:269:ARG:HA	1:A:280:GLN:HG2	1.83	0.61
1:D:143:LEU:HD23	1:D:149:LEU:HB2	1.82	0.61
1:F:242:LYS:HB2	1:F:244:LEU:HD13	1.83	0.61
1:J:91:VAL:HG11	1:K:111:GLN:NE2	2.15	0.61
1:K:280:GLN:O	1:K:280:GLN:HG3	2.00	0.61
1:H:319:PHE:CZ	1:G:315:LEU:HD21	2.33	0.61
1:D:215:ASN:ND2	1:D:451:HIS:HD2	1.99	0.61
1:D:304:LEU:HD22	1:D:324:ILE:HG22	1.82	0.61
3:D:1001:ADP:H5'2	3:D:1001:ADP:C8	2.35	0.61
1:E:57:VAL:HA	1:E:104:PRO:HG2	1.83	0.61
1:I:396:VAL:HG22	1:I:396:VAL:O	2.01	0.61
1:K:553:PRO:O	1:K:556:ARG:HG2	2.01	0.61
1:H:397:LEU:HB3	1:G:401:PRO:HB2	1.83	0.61
1:E:291:PHE:HB2	1:E:436:PRO:HG3	1.81	0.61
1:J:189:SER:O	1:J:194:ARG:NH2	2.33	0.61
1:L:597:ARG:HB3	1:L:600:GLU:HG3	1.81	0.61
1:A:76:GLU:HG3	1:B:19:LEU:HD21	1.83	0.61
1:E:474:GLU:OE1	1:E:511:ARG:NH2	2.34	0.61
1:E:553:PRO:HA	1:E:556:ARG:HD3	1.81	0.61
1:G:142:LEU:HG	1:G:252:LEU:HD11	1.83	0.61
1:I:323:ASN:HD22	1:I:397:LEU:HD23	1.65	0.61
1:K:184:HIS:ND1	1:K:594:TRP:CZ3	2.69	0.61
1:A:349:PHE:CE1	1:A:356:PRO:HB3	2.36	0.60
1:L:358:ASN:OD1	1:L:358:ASN:O	2.19	0.60
1:I:30:TRP:CE2	1:I:96:ARG:HG3	2.36	0.60
1:L:193:ASP:N	1:L:206:THR:OG1	2.34	0.60
1:B:308:PHE:CD2	1:B:410:ARG:HD3	2.36	0.60
1:C:530:GLU:OE2	1:C:532:ARG:HD3	2.02	0.60
1:F:291:PHE:HB2	1:F:436:PRO:HG3	1.83	0.60
1:J:87:LEU:H	1:J:87:LEU:CD1	2.14	0.60
1:E:219:GLU:OE1	1:E:283:GLN:HG3	2.01	0.60
1:K:297:GLU:OE1	1:K:301:ARG:HD3	2.02	0.60
1:L:47:VAL:HB	1:L:116:VAL:HG22	1.83	0.60
1:H:219:GLU:OE1	1:H:283:GLN:HG3	2.02	0.60
1:E:175:LYS:NZ	1:E:524:GLN:HA	2.15	0.60
1:F:547:LEU:HD12	1:F:547:LEU:H	1.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:406:ALA:HA	1:G:409:ARG:HG2	1.84	0.60
1:K:174:THR:HG22	3:K:1001:ADP:H5'2	1.83	0.60
1:L:376:ILE:CD1	1:L:411:LEU:HB3	2.26	0.60
1:B:530:GLU:OE2	1:B:532:ARG:HD3	2.01	0.60
1:C:310:ASP:OD2	1:C:314:SER:HB3	2.02	0.60
1:K:213:ILE:HD13	1:K:221:LEU:HD22	1.83	0.60
1:A:173:ALA:O	3:A:1001:ADP:O1B	2.20	0.60
1:E:175:LYS:NZ	1:E:524:GLN:CA	2.63	0.60
1:K:414:VAL:HG22	1:K:414:VAL:O	2.02	0.60
1:D:269:ARG:HA	1:D:280:GLN:HG2	1.82	0.60
1:E:218:GLY:O	1:F:202:ARG:NH1	2.35	0.60
1:I:299:CYS:HB2	1:I:332:ALA:HB2	1.83	0.60
1:K:530:GLU:HG3	1:K:532:ARG:H	1.66	0.60
1:H:249:TYR:OH	1:H:591:PHE:O	2.17	0.60
1:A:371:THR:OG1	1:A:373:GLU:OE1	2.19	0.60
1:C:473:LYS:NZ	1:C:480:ASP:O	2.30	0.60
1:F:156:ILE:HA	1:F:162:GLY:O	2.02	0.60
1:G:17:MET:HE1	1:I:83:VAL:HG21	1.84	0.60
1:A:142:LEU:HD12	1:A:248:ARG:HB3	1.83	0.59
1:B:371:THR:HG23	1:B:374:GLN:HG3	1.82	0.59
1:B:414:VAL:HG22	1:B:414:VAL:O	2.02	0.59
1:K:398:LYS:O	1:K:398:LYS:HG2	2.01	0.59
1:B:73:VAL:HG23	1:B:73:VAL:O	2.02	0.59
1:E:154:ARG:HG2	1:E:154:ARG:HH11	1.67	0.59
1:K:228:ASN:OD1	1:K:231:MET:N	2.34	0.59
1:A:156:ILE:HD13	1:A:164:ILE:HD11	1.84	0.59
1:F:153:PHE:HD2	1:F:195:THR:HG21	1.67	0.59
1:J:282:ASP:HB2	1:K:202:ARG:HH12	1.62	0.59
1:K:495:ARG:NH2	1:K:527:SER:HA	2.17	0.59
1:D:441:ARG:HH21	1:D:441:ARG:CG	2.15	0.59
1:G:192:MET:HE1	1:G:209:GLY:HA3	1.83	0.59
1:J:154:ARG:NH1	1:J:159:GLU:OE2	2.35	0.59
1:J:385:GLU:O	1:J:385:GLU:HG2	2.02	0.59
1:K:282:ASP:N	1:K:282:ASP:OD1	2.33	0.59
1:L:553:PRO:HA	1:L:556:ARG:HD3	1.83	0.59
1:H:147:GLN:HA	1:H:147:GLN:HE21	1.67	0.59
1:F:163:HIS:CE1	1:F:509:ALA:HA	2.37	0.59
1:F:453:LEU:HB3	1:F:457:ALA:HB3	1.84	0.59
1:B:473:LYS:HG2	1:B:517:ILE:HD11	1.85	0.59
1:B:553:PRO:O	1:B:556:ARG:HG2	2.02	0.59
1:J:163:HIS:HB3	1:J:519:LEU:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:335:GLN:NE2	1:C:343:ILE:O	2.36	0.59
1:G:323:ASN:OD1	1:I:405:ARG:CD	2.50	0.59
1:I:192:MET:HA	1:I:195:THR:HG22	1.84	0.59
1:J:323:ASN:OD1	1:J:397:LEU:HD22	2.02	0.59
1:B:302:ARG:NH1	1:B:325:GLU:OE2	2.29	0.59
1:E:192:MET:HE1	1:E:209:GLY:HA3	1.83	0.59
1:K:473:LYS:CB	1:K:517:ILE:HD11	2.32	0.59
1:L:603:ASP:OD1	1:L:603:ASP:N	2.35	0.59
1:H:142:LEU:HG	1:H:252:LEU:HD11	1.84	0.59
1:C:202:ARG:HH21	1:C:202:ARG:CG	2.16	0.59
1:D:162:GLY:HA3	1:D:538:ALA:HB3	1.85	0.59
1:J:142:LEU:HG	1:J:252:LEU:HD11	1.84	0.59
1:J:264:LEU:HD23	1:J:447:VAL:HB	1.83	0.59
1:K:597:ARG:HG2	1:K:600:GLU:CD	2.27	0.59
1:H:188:ARG:NH2	1:H:260:ARG:HG2	2.17	0.59
1:A:163:HIS:HB3	1:A:519:LEU:O	2.03	0.59
1:G:106:ASN:HB3	1:G:108:ILE:HG23	1.84	0.59
1:I:419:SER:N	1:I:420:PRO:HD2	2.18	0.59
1:I:560:GLN:HA	1:I:563:ARG:HG3	1.84	0.59
1:J:324:ILE:HD13	1:J:407:PHE:CZ	2.36	0.59
1:K:277:ILE:HD11	1:K:426:LEU:HD22	1.83	0.59
1:L:228:ASN:ND2	1:L:600:GLU:OE1	2.36	0.59
1:B:57:VAL:HA	1:B:104:PRO:HG2	1.85	0.58
1:C:70:HIS:HB2	1:D:20:GLY:HA3	1.85	0.58
1:K:353:GLU:OE1	1:K:353:GLU:HA	2.03	0.58
1:L:412:ARG:HH11	1:L:415:GLN:HE22	1.50	0.58
1:B:331:LEU:HD21	1:B:344:VAL:HG12	1.85	0.58
1:G:228:ASN:ND2	1:G:600:GLU:OE2	2.36	0.58
1:K:473:LYS:CA	1:K:473:LYS:HZ2	2.16	0.58
1:C:173:ALA:O	3:C:1001:ADP:O1B	2.21	0.58
1:E:548:ALA:HB2	1:F:556:ARG:HB2	1.85	0.58
1:K:267:PRO:HG3	1:K:453:LEU:HD21	1.84	0.58
1:H:418:LEU:HD23	1:H:421:LEU:HD12	1.85	0.58
1:A:24:VAL:CG1	1:A:110:PRO:HD2	2.34	0.58
1:D:453:LEU:HB3	1:D:457:ALA:HB3	1.84	0.58
1:E:553:PRO:O	1:E:556:ARG:HG2	2.03	0.58
1:G:453:LEU:HB3	1:G:457:ALA:HB3	1.85	0.58
1:K:149:LEU:HD13	1:K:585:VAL:HG21	1.84	0.58
1:K:149:LEU:HD22	1:K:587:VAL:HG11	1.84	0.58
1:K:399:GLN:HB3	1:K:404:LEU:HD21	1.86	0.58
1:K:473:LYS:CB	1:K:473:LYS:HZ2	2.17	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:153:PHE:HD2	1:H:195:THR:HG21	1.68	0.58
1:H:354:THR:CG2	1:H:355:PRO:HD2	2.33	0.58
1:B:223:PHE:H	1:B:284:ARG:HH11	1.50	0.58
1:K:450:ILE:HD12	1:K:458:GLN:HB3	1.84	0.58
1:L:267:PRO:HB3	1:L:421:LEU:HD21	1.85	0.58
1:H:149:LEU:CD2	1:H:587:VAL:HG11	2.32	0.58
1:B:213:ILE:CG2	1:B:447:VAL:HG22	2.33	0.58
1:B:547:LEU:H	1:B:547:LEU:HD12	1.67	0.58
1:D:70:HIS:HB2	1:E:20:GLY:HA3	1.84	0.58
1:E:359:LEU:CD2	1:E:374:GLN:NE2	2.66	0.58
1:K:138:PHE:CB	1:K:191:VAL:HG11	2.34	0.58
1:K:174:THR:HB	3:K:1001:ADP:C5'	2.32	0.58
1:K:309:SER:OG	1:K:501:ILE:CG2	2.51	0.58
1:K:472:TYR:CE1	1:K:476:VAL:CB	2.87	0.58
1:L:343:ILE:HD13	1:L:362:SER:HB2	1.84	0.58
1:C:530:GLU:HG3	1:C:532:ARG:H	1.69	0.58
1:I:149:LEU:HD13	1:I:585:VAL:HG21	1.86	0.58
1:I:51:LYS:HZ3	1:I:106:ASN:HD21	1.50	0.58
1:I:163:HIS:N	1:I:163:HIS:CD2	2.72	0.58
1:A:202:ARG:O	1:A:204:SER:OG	2.17	0.58
1:J:403:THR:N	1:K:319:PHE:CE1	2.72	0.58
1:C:598:ARG:O	1:C:601:VAL:HG12	2.03	0.58
1:E:131:ASP:OD1	1:E:131:ASP:N	2.35	0.58
1:G:101:ARG:HD3	1:G:126:MET:O	2.03	0.58
1:G:170:SER:HA	3:G:1001:ADP:O2B	2.03	0.58
1:G:597:ARG:CG	1:G:600:GLU:HG3	2.34	0.58
1:L:202:ARG:HH21	1:L:478:ARG:HH22	1.51	0.58
1:B:166:ILE:HG22	1:B:175:LYS:HB3	1.86	0.57
1:D:161:GLY:HA3	1:D:513:ARG:HE	1.64	0.57
1:E:597:ARG:NH2	1:E:599:ASP:OD2	2.37	0.57
1:L:473:LYS:HE3	1:L:515:LEU:O	2.04	0.57
1:C:212:LEU:HD13	1:C:438:PRO:HB3	1.87	0.57
1:I:588:ASN:ND2	1:I:588:ASN:O	2.37	0.57
1:L:553:PRO:O	1:L:556:ARG:HG2	2.04	0.57
1:H:495:ARG:NH2	1:H:554:GLU:OE2	2.37	0.57
1:A:135:GLU:O	1:A:194:ARG:HD2	2.04	0.57
1:B:163:HIS:N	1:B:163:HIS:CD2	2.73	0.57
1:D:153:PHE:HD2	1:D:195:THR:HG21	1.70	0.57
1:D:163:HIS:N	1:D:163:HIS:CD2	2.73	0.57
1:D:175:LYS:CG	3:D:1001:ADP:O1B	2.47	0.57
1:E:263:GLN:HE21	1:E:265:LEU:HD21	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:530:GLU:OE2	1:E:532:ARG:HD3	2.02	0.57
1:J:238:VAL:HG11	1:J:248:ARG:NH2	2.18	0.57
1:J:354:THR:HG23	1:J:381:TYR:CZ	2.39	0.57
1:L:33:VAL:HG21	1:L:93:TYR:CD2	2.39	0.57
1:H:163:HIS:CD2	1:H:163:HIS:N	2.71	0.57
1:H:242:LYS:HZ3	1:H:588:ASN:ND2	2.03	0.57
1:B:268:PRO:HG3	1:B:292:VAL:CG1	2.34	0.57
1:B:470:PHE:CE1	1:B:515:LEU:CD2	2.87	0.57
1:C:269:ARG:HA	1:C:280:GLN:HG2	1.86	0.57
1:D:291:PHE:HB2	1:D:436:PRO:HG3	1.85	0.57
1:E:166:ILE:HG23	1:E:541:VAL:HB	1.86	0.57
1:F:103:ASP:HB3	1:F:104:PRO:HD3	1.86	0.57
1:F:601:VAL:HG13	1:F:601:VAL:O	2.04	0.57
1:I:87:LEU:HD12	1:I:88:PRO:HD3	1.71	0.57
1:K:560:GLN:HA	1:K:563:ARG:HG3	1.86	0.57
1:H:388:GLU:HG2	1:E:388:GLU:HB3	1.85	0.57
1:D:201:GLY:N	1:D:204:SER:OG	2.37	0.57
1:D:215:ASN:HD21	1:D:451:HIS:HD2	1.51	0.57
1:E:327:LYS:HZ2	1:E:394:LYS:HG2	1.69	0.57
1:J:402:GLY:C	1:K:319:PHE:HD1	2.11	0.57
1:B:149:LEU:HD22	1:B:587:VAL:HG11	1.87	0.57
1:C:315:LEU:HD22	1:D:319:PHE:CZ	2.37	0.57
1:I:162:GLY:H	1:I:538:ALA:HB2	1.69	0.57
1:J:64:ASP:OD2	1:J:98:LEU:HD21	2.05	0.57
1:C:597:ARG:HG3	1:C:600:GLU:HG3	1.86	0.57
1:E:149:LEU:HD23	1:E:587:VAL:HG11	1.86	0.57
1:E:269:ARG:HA	1:E:280:GLN:HG2	1.86	0.57
1:I:71:GLU:HG3	1:I:92:SER:HB3	1.86	0.57
1:L:474:GLU:OE1	1:L:511:ARG:NH2	2.38	0.57
1:B:231:MET:HE3	1:B:232:VAL:HG13	1.86	0.57
1:B:548:ALA:HB2	1:C:556:ARG:HB2	1.87	0.57
1:J:149:LEU:HD21	1:J:576:VAL:HG21	1.87	0.57
1:K:19:LEU:HD13	1:K:32:ALA:HB2	1.87	0.57
1:H:163:HIS:CD2	1:H:163:HIS:H	2.20	0.57
1:A:530:GLU:HG3	1:A:532:ARG:H	1.69	0.57
1:D:103:ASP:CB	1:D:104:PRO:CD	2.64	0.57
1:D:238:VAL:HG11	1:D:248:ARG:HH21	1.67	0.57
1:D:335:GLN:NE2	1:D:343:ILE:O	2.37	0.57
1:E:327:LYS:NZ	1:E:394:LYS:HG2	2.19	0.57
1:I:131:ASP:OD1	1:I:131:ASP:N	2.38	0.57
1:C:211:ALA:N	1:C:444:GLN:O	2.33	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:161:GLY:N	1:D:513:ARG:HH21	2.03	0.56
1:I:41:LEU:O	1:I:63:VAL:CG1	2.29	0.56
1:J:41:LEU:HB2	1:K:107:PHE:HB2	1.86	0.56
1:J:51:LYS:HG2	1:J:52:PRO:HD2	1.87	0.56
1:K:309:SER:OG	1:K:501:ILE:HG22	2.05	0.56
1:L:192:MET:HE1	1:L:209:GLY:HA3	1.86	0.56
1:L:307:VAL:HG13	1:L:414:VAL:HG11	1.85	0.56
1:E:51:LYS:HG2	1:E:52:PRO:HD2	1.87	0.56
1:E:174:THR:CG2	3:E:1001:ADP:H5'2	2.34	0.56
1:G:24:VAL:HG11	1:G:110:PRO:O	2.04	0.56
1:I:414:VAL:O	1:I:414:VAL:HG22	2.05	0.56
1:I:553:PRO:O	1:I:556:ARG:HG2	2.03	0.56
1:K:349:PHE:N	1:K:349:PHE:CD1	2.72	0.56
1:K:472:TYR:C	1:K:472:TYR:CD1	2.84	0.56
1:A:163:HIS:N	1:A:163:HIS:CD2	2.73	0.56
1:A:553:PRO:HA	1:A:556:ARG:HD3	1.88	0.56
1:B:213:ILE:HG23	1:B:447:VAL:HG22	1.87	0.56
1:B:238:VAL:HG11	1:B:248:ARG:HH21	1.71	0.56
1:D:263:GLN:CB	1:D:443:ILE:HG21	2.35	0.56
1:E:151:LEU:HD21	1:E:156:ILE:HD11	1.87	0.56
1:E:264:LEU:HD23	1:E:447:VAL:HB	1.88	0.56
1:G:103:ASP:HB3	1:G:104:PRO:CD	2.27	0.56
1:G:168:GLY:O	1:G:175:LYS:NZ	2.35	0.56
1:K:164:ILE:CD1	1:K:182:LEU:HD13	2.35	0.56
1:K:400:SER:OG	1:K:403:THR:OG1	2.19	0.56
1:A:238:VAL:HG11	1:A:248:ARG:NH2	2.20	0.56
1:E:547:LEU:H	1:E:547:LEU:HD12	1.69	0.56
1:L:122:ARG:O	1:L:126:MET:HG2	2.05	0.56
1:A:335:GLN:NE2	1:A:343:ILE:O	2.38	0.56
1:D:70:HIS:CG	1:D:73:VAL:HG21	2.39	0.56
1:E:249:TYR:HE1	1:E:590:PRO:CB	2.18	0.56
1:G:553:PRO:O	1:G:556:ARG:HG2	2.06	0.56
1:B:218:GLY:HA2	1:B:451:HIS:CB	2.35	0.56
1:D:406:ALA:HA	1:D:409:ARG:HG2	1.87	0.56
1:K:70:HIS:HB3	1:K:73:VAL:HG22	1.87	0.56
1:K:255:PRO:HB2	1:K:257:GLU:HG2	1.86	0.56
1:A:547:LEU:HD12	1:A:547:LEU:H	1.71	0.56
1:B:437:ASP:HB3	1:B:440:ARG:HB2	1.86	0.56
1:E:163:HIS:CD2	1:E:163:HIS:N	2.73	0.56
1:F:163:HIS:CD2	1:F:163:HIS:N	2.73	0.56
1:G:156:ILE:HD13	1:G:164:ILE:HD11	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:601:VAL:O	1:J:601:VAL:HG13	2.05	0.56
1:K:163:HIS:CD2	1:K:163:HIS:N	2.72	0.56
1:K:188:ARG:HH11	1:K:188:ARG:CG	2.19	0.56
1:L:75:PHE:O	1:L:79:VAL:HG23	2.05	0.56
1:L:355:PRO:N	1:L:355:PRO:C	2.58	0.56
1:B:163:HIS:HB3	1:B:519:LEU:O	2.06	0.56
1:B:473:LYS:HB3	1:B:515:LEU:HG	1.88	0.56
1:E:138:PHE:CZ	1:E:151:LEU:HD23	2.40	0.56
1:K:363:GLU:OE1	1:K:363:GLU:N	2.32	0.56
1:K:470:PHE:HD1	1:K:517:ILE:HD12	1.70	0.56
1:B:406:ALA:HA	1:B:409:ARG:HG2	1.88	0.56
1:D:194:ARG:O	1:D:197:GLN:HB2	2.06	0.56
1:D:530:GLU:HG3	1:D:532:ARG:H	1.71	0.56
1:F:530:GLU:OE2	1:F:532:ARG:HD3	2.06	0.56
1:D:76:GLU:HA	1:E:21:THR:HG21	1.88	0.56
1:J:101:ARG:NH1	1:J:126:MET:HA	2.21	0.56
1:J:597:ARG:HG2	1:J:600:GLU:HG3	1.87	0.56
1:L:269:ARG:HA	1:L:280:GLN:HG2	1.88	0.56
1:B:295:ILE:HD13	1:B:422:ILE:CG2	2.33	0.55
1:J:385:GLU:HA	1:J:389:GLY:HA2	1.88	0.55
1:K:215:ASN:HA	1:K:221:LEU:HD13	1.86	0.55
1:H:163:HIS:HB3	1:H:519:LEU:O	2.05	0.55
1:H:335:GLN:NE2	1:H:343:ILE:O	2.38	0.55
1:C:188:ARG:NH2	1:C:259:PHE:HA	2.21	0.55
1:G:530:GLU:OE2	1:G:532:ARG:HD3	2.06	0.55
1:I:107:PHE:HB2	1:K:41:LEU:HB2	1.88	0.55
1:B:299:CYS:O	1:B:329:PHE:HA	2.07	0.55
3:B:1001:ADP:O1A	3:B:1001:ADP:H3'	2.05	0.55
1:E:174:THR:HG22	3:E:1001:ADP:C4'	2.36	0.55
1:F:163:HIS:HE1	1:F:508:ILE:O	1.88	0.55
1:I:352:SER:OG	1:I:354:THR:OG1	2.24	0.55
1:H:547:LEU:H	1:H:547:LEU:HD12	1.72	0.55
1:D:161:GLY:HA3	1:D:513:ARG:NH2	2.19	0.55
1:D:215:ASN:HD21	1:D:219:GLU:HA	1.72	0.55
1:E:249:TYR:CE1	1:E:590:PRO:HB3	2.42	0.55
1:E:376:ILE:HD13	1:E:411:LEU:HB3	1.88	0.55
1:F:142:LEU:HD22	1:F:146:GLY:HA2	1.87	0.55
1:J:248:ARG:HH11	1:J:590:PRO:HA	1.70	0.55
1:L:236:ASP:O	1:L:240:ARG:HG2	2.06	0.55
1:B:501:ILE:O	1:B:504:VAL:HG12	2.07	0.55
1:G:156:ILE:O	1:G:162:GLY:O	2.24	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:17:MET:HE2	1:I:113:GLY:O	2.07	0.55
1:K:490:ASN:OD1	1:K:490:ASN:C	2.50	0.55
1:L:530:GLU:OE2	1:L:532:ARG:HD3	2.07	0.55
1:L:547:LEU:H	1:L:547:LEU:HD12	1.72	0.55
1:D:161:GLY:HA3	1:D:513:ARG:NE	2.22	0.55
1:D:219:GLU:OE2	1:D:223:PHE:CZ	2.60	0.55
1:J:403:THR:N	1:K:319:PHE:HE1	2.03	0.55
1:A:149:LEU:CD2	1:A:576:VAL:HG21	2.37	0.55
1:B:75:PHE:CD1	1:C:71:GLU:CG	2.89	0.55
1:D:219:GLU:OE2	1:D:223:PHE:CE2	2.60	0.55
1:J:231:MET:CE	1:J:256:ALA:HB1	2.24	0.55
1:K:298:PHE:C	1:K:298:PHE:CD1	2.85	0.55
1:L:219:GLU:HA	1:L:222:LEU:HD13	1.88	0.55
1:C:291:PHE:HB2	1:C:436:PRO:HG3	1.87	0.55
1:E:352:SER:HB3	1:E:354:THR:HG22	1.89	0.55
1:H:38:SER:HB3	1:L:52:PRO:HG3	1.89	0.55
1:H:546:ASP:HB3	1:H:549:GLU:HG2	1.89	0.55
1:D:560:GLN:HA	1:D:563:ARG:HG3	1.88	0.55
1:J:248:ARG:HB2	1:J:590:PRO:HG3	1.89	0.55
1:L:153:PHE:HD2	1:L:195:THR:HG21	1.71	0.55
1:H:223:PHE:CD1	1:H:601:VAL:CG2	2.80	0.55
1:A:355:PRO:HB2	1:A:357:GLU:OE1	2.06	0.55
1:C:547:LEU:H	1:C:547:LEU:HD12	1.72	0.55
1:D:546:ASP:HB3	1:D:549:GLU:HG2	1.89	0.55
1:K:247:ASP:C	1:K:251:LEU:HD13	2.32	0.55
1:A:215:ASN:HD21	1:A:219:GLU:H	1.55	0.54
1:B:62:LEU:HD23	1:B:63:VAL:O	2.07	0.54
1:B:419:SER:N	1:B:420:PRO:HD2	2.21	0.54
1:G:166:ILE:CG2	1:G:175:LYS:HB3	2.37	0.54
1:I:298:PHE:CD1	1:I:298:PHE:C	2.85	0.54
1:H:310:ASP:OD2	1:H:314:SER:HB3	2.06	0.54
1:A:155:PHE:CD2	1:A:579:PRO:CG	2.78	0.54
1:B:213:ILE:HD11	1:B:221:LEU:HD11	1.89	0.54
1:B:238:VAL:HG11	1:B:248:ARG:NH2	2.22	0.54
1:F:41:LEU:HD13	1:F:66:VAL:HG12	1.89	0.54
1:F:566:ALA:HA	1:F:569:LEU:CG	2.37	0.54
1:A:155:PHE:CE2	1:A:579:PRO:CB	2.90	0.54
1:C:64:ASP:OD1	1:C:96:ARG:HD2	2.07	0.54
1:I:349:PHE:CD2	1:I:349:PHE:N	2.75	0.54
1:H:149:LEU:HD12	1:H:150:PRO:CD	2.38	0.54
1:B:79:VAL:HG21	1:C:19:LEU:HD12	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:149:LEU:HD13	1:G:585:VAL:HG21	1.88	0.54
1:I:478:ARG:HG3	1:I:516:GLY:HA3	1.90	0.54
1:K:135:GLU:O	1:K:194:ARG:NH1	2.40	0.54
1:K:280:GLN:HG2	1:K:452:ALA:HB1	1.89	0.54
1:H:219:GLU:OE1	1:H:283:GLN:CG	2.55	0.54
1:A:174:THR:CB	3:A:1001:ADP:H5'2	2.37	0.54
1:B:192:MET:HE1	1:B:209:GLY:HA3	1.89	0.54
1:B:219:GLU:CA	1:B:222:LEU:HD11	2.21	0.54
1:D:155:PHE:HA	1:D:161:GLY:O	2.07	0.54
1:F:180:LEU:HD11	1:F:221:LEU:HD21	1.89	0.54
1:G:71:GLU:HG3	1:G:92:SER:HB3	1.89	0.54
1:L:354:THR:OG1	1:L:355:PRO:HD3	2.03	0.54
1:H:315:LEU:HG	1:H:316:ASN:N	2.22	0.54
1:B:460:PHE:C	1:B:460:PHE:CD1	2.85	0.54
1:J:324:ILE:HD11	1:J:383:LEU:HD21	1.89	0.54
1:B:201:GLY:HA2	1:B:204:SER:OG	2.08	0.54
1:E:149:LEU:HD22	1:E:587:VAL:HG11	1.89	0.54
1:G:469:VAL:O	1:G:473:LYS:HG2	2.08	0.54
1:I:24:VAL:HG11	1:I:110:PRO:O	2.07	0.54
1:A:155:PHE:CA	1:A:161:GLY:HA3	2.34	0.54
1:A:263:GLN:HE21	1:A:265:LEU:HD21	1.72	0.54
1:J:41:LEU:HB2	1:K:107:PHE:CB	2.37	0.54
1:L:371:THR:OG1	1:L:373:GLU:OE1	2.25	0.54
1:H:20:GLY:HA3	1:G:70:HIS:HB2	1.90	0.54
1:A:192:MET:HA	1:A:195:THR:HG22	1.90	0.54
1:E:473:LYS:HG3	1:E:517:ILE:CG1	2.37	0.54
1:J:149:LEU:HD13	1:J:585:VAL:HG21	1.90	0.54
1:K:172:VAL:HG11	1:K:544:ARG:HD2	1.89	0.54
1:H:42:ASP:OD2	1:H:586:LEU:HD22	2.08	0.54
1:H:474:GLU:OE1	1:H:511:ARG:NH2	2.39	0.54
1:A:149:LEU:CD1	1:A:585:VAL:HG21	2.37	0.54
1:B:268:PRO:HD2	1:B:421:LEU:HD23	1.90	0.54
1:B:292:VAL:HG21	1:B:426:LEU:CD1	2.38	0.54
1:D:597:ARG:HB2	1:D:600:GLU:HG3	1.89	0.54
1:I:98:LEU:HD23	1:I:583:ASN:OD1	2.07	0.54
1:I:397:LEU:HD22	1:I:397:LEU:H	1.72	0.54
1:J:158:GLY:O	1:J:513:ARG:NH2	2.40	0.54
1:J:218:GLY:HA2	1:J:451:HIS:CG	2.43	0.54
1:J:283:GLN:NE2	1:J:598:ARG:HD3	2.23	0.54
1:K:473:LYS:CB	1:K:473:LYS:NZ	2.71	0.54
1:K:597:ARG:HG2	1:K:600:GLU:CG	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:238:VAL:HG11	1:H:248:ARG:NH2	2.18	0.53
1:B:252:LEU:HD22	1:B:254:LEU:HD12	1.91	0.53
1:E:174:THR:O	1:E:174:THR:OG1	2.25	0.53
1:I:57:VAL:HA	1:I:104:PRO:HG2	1.90	0.53
1:L:263:GLN:HE21	1:L:265:LEU:HD21	1.73	0.53
1:C:215:ASN:HB3	1:C:449:ASP:HA	1.89	0.53
1:F:560:GLN:HA	1:F:563:ARG:HG3	1.90	0.53
1:G:230:ARG:O	1:G:233:GLU:HG2	2.07	0.53
1:I:63:VAL:HG12	1:I:63:VAL:O	2.07	0.53
1:K:324:ILE:CD1	1:K:324:ILE:N	2.72	0.53
1:L:164:ILE:HG12	1:L:539:ILE:HB	1.90	0.53
1:A:453:LEU:HB3	1:A:457:ALA:HB3	1.89	0.53
1:D:64:ASP:OD1	1:D:96:ARG:HD2	2.08	0.53
1:E:173:ALA:HB2	1:E:544:ARG:N	2.23	0.53
1:E:405:ARG:HD2	1:F:323:ASN:OD1	2.08	0.53
1:G:269:ARG:HB2	1:G:278:VAL:HG23	1.89	0.53
1:K:372:PHE:CE2	1:K:376:ILE:HD11	2.43	0.53
1:L:131:ASP:OD1	1:L:131:ASP:N	2.39	0.53
1:I:174:THR:O	1:I:174:THR:OG1	2.21	0.53
1:I:530:GLU:OE2	1:I:532:ARG:HD3	2.08	0.53
1:K:235:GLU:OE1	1:K:248:ARG:HD3	2.08	0.53
1:L:33:VAL:HG21	1:L:93:TYR:CG	2.44	0.53
1:H:373:GLU:HG3	1:H:415:GLN:NE2	2.24	0.53
1:H:423:ARG:NH1	1:H:426:LEU:HD21	2.23	0.53
1:E:342:LEU:HB3	1:E:369:LEU:HD12	1.90	0.53
1:I:268:PRO:HG3	1:I:292:VAL:HG12	1.89	0.53
1:I:532:ARG:O	1:I:536:ASN:ND2	2.34	0.53
1:K:211:ALA:HB3	1:K:445:LEU:HD12	1.90	0.53
1:H:76:GLU:HA	1:L:21:THR:HG21	1.90	0.53
1:H:228:ASN:ND2	1:H:600:GLU:HB3	2.24	0.53
1:B:223:PHE:HA	1:B:284:ARG:HH11	1.67	0.53
1:D:79:VAL:HG21	1:E:19:LEU:HD12	1.89	0.53
1:D:392:ASP:HB3	1:D:395:TRP:HB2	1.90	0.53
1:F:553:PRO:HA	1:F:556:ARG:HD3	1.89	0.53
1:I:597:ARG:NH2	1:I:599:ASP:OD2	2.41	0.53
1:K:164:ILE:HG12	1:K:539:ILE:HB	1.90	0.53
1:K:298:PHE:HD2	1:K:422:ILE:HD13	1.74	0.53
1:L:135:GLU:OE2	1:L:154:ARG:NH2	2.42	0.53
1:H:506:LEU:HD23	1:H:533:ILE:CD1	2.39	0.53
1:C:41:LEU:HB2	1:D:107:PHE:CB	2.39	0.53
1:C:174:THR:HG22	3:C:1001:ADP:H5'2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:213:ILE:HD13	1:E:221:LEU:HD22	1.91	0.53
1:E:310:ASP:OD2	1:E:314:SER:HB3	2.07	0.53
1:E:560:GLN:HA	1:E:563:ARG:HG3	1.90	0.53
1:G:248:ARG:HH11	1:G:590:PRO:HA	1.74	0.53
1:J:71:GLU:OE2	1:L:76:GLU:HB3	2.09	0.53
1:C:231:MET:SD	1:C:249:TYR:HE2	2.32	0.53
1:D:441:ARG:HH21	1:D:441:ARG:HG3	1.74	0.53
1:I:70:HIS:CE1	1:I:82:VAL:HG11	2.44	0.53
1:I:400:SER:OG	1:I:401:PRO:CD	2.57	0.53
1:B:175:LYS:N	3:B:1001:ADP:O1B	2.42	0.53
1:E:219:GLU:OE1	1:E:283:GLN:CB	2.56	0.53
1:G:388:GLU:O	1:G:388:GLU:HG2	2.09	0.53
1:I:142:LEU:C	1:I:588:ASN:HD21	2.16	0.53
1:J:566:ALA:HA	1:J:569:LEU:CG	2.35	0.53
1:L:162:GLY:HA3	1:L:513:ARG:HG2	1.91	0.53
1:H:153:PHE:CD2	1:H:195:THR:HG21	2.44	0.53
1:A:155:PHE:CE2	1:A:579:PRO:CG	2.91	0.53
1:A:157:ASN:HD21	1:A:159:GLU:HG3	1.74	0.53
1:A:219:GLU:OE2	1:A:283:GLN:HB2	2.08	0.53
1:B:263:GLN:HE21	1:B:265:LEU:HD21	1.73	0.53
1:D:473:LYS:NZ	1:D:480:ASP:O	2.30	0.53
1:H:530:GLU:OE2	1:H:532:ARG:HD3	2.09	0.52
1:C:180:LEU:HD11	1:C:221:LEU:HD21	1.89	0.52
1:D:24:VAL:O	1:D:109:PRO:HB3	2.09	0.52
1:F:553:PRO:O	1:F:556:ARG:HG2	2.09	0.52
1:J:112:PRO:HB2	1:L:70:HIS:CE1	2.44	0.52
1:J:156:ILE:HA	1:J:162:GLY:O	2.08	0.52
1:J:282:ASP:HB3	1:K:202:ARG:CZ	2.38	0.52
1:K:41:LEU:HD13	1:K:66:VAL:HG12	1.90	0.52
1:K:473:LYS:CD	1:K:515:LEU:O	2.53	0.52
1:L:129:SER:HB3	1:L:132:LYS:HG3	1.90	0.52
1:H:223:PHE:HZ	1:H:598:ARG:HD3	1.71	0.52
1:H:553:PRO:O	1:H:556:ARG:HG2	2.08	0.52
1:B:213:ILE:CD1	1:B:221:LEU:HD11	2.40	0.52
1:C:76:GLU:OE2	1:D:92:SER:HB2	2.09	0.52
1:D:248:ARG:NH1	1:D:589:TYR:O	2.41	0.52
1:J:76:GLU:HG3	1:K:19:LEU:HD21	1.92	0.52
1:J:218:GLY:HA2	1:J:451:HIS:HB2	1.91	0.52
1:J:379:LEU:O	1:J:383:LEU:HB2	2.09	0.52
1:J:598:ARG:O	1:J:601:VAL:CG1	2.50	0.52
1:K:175:LYS:NZ	1:K:524:GLN:HA	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:388:GLU:CG	1:E:388:GLU:CG	2.87	0.52
1:C:472:TYR:CE2	1:C:476:VAL:HG11	2.44	0.52
1:I:59:PHE:CE1	1:I:110:PRO:HG3	2.44	0.52
1:I:263:GLN:HE21	1:I:265:LEU:HD21	1.74	0.52
1:K:453:LEU:HD23	1:K:453:LEU:N	2.23	0.52
1:L:396:VAL:O	1:L:399:GLN:HB2	2.08	0.52
1:H:423:ARG:HH11	1:H:426:LEU:HD21	1.74	0.52
1:D:267:PRO:HB3	1:D:421:LEU:HD21	1.92	0.52
1:E:154:ARG:HG2	1:E:154:ARG:NH1	2.25	0.52
1:J:42:ASP:OD2	1:J:586:LEU:HD22	2.09	0.52
1:J:101:ARG:NH2	1:J:131:ASP:OD2	2.42	0.52
1:J:155:PHE:HA	1:J:161:GLY:HA3	1.92	0.52
1:L:588:ASN:N	1:L:588:ASN:HD22	2.08	0.52
1:B:184:HIS:CE1	1:B:188:ARG:HG3	2.45	0.52
1:B:193:ASP:OD2	1:B:206:THR:HG21	2.09	0.52
1:E:441:ARG:HD2	1:E:442:GLY:H	1.74	0.52
1:K:155:PHE:CA	1:K:161:GLY:HA3	2.37	0.52
1:A:228:ASN:ND2	1:A:600:GLU:HB3	2.25	0.52
1:B:393:PRO:HA	1:B:396:VAL:HG12	1.92	0.52
1:B:405:ARG:HH22	1:C:326:GLU:HG2	1.74	0.52
1:D:547:LEU:H	1:D:547:LEU:HD12	1.75	0.52
1:G:283:GLN:NE2	1:G:598:ARG:HB2	2.25	0.52
1:G:474:GLU:OE1	1:G:511:ARG:NH2	2.39	0.52
1:I:73:VAL:HG12	1:I:82:VAL:HG21	1.91	0.52
1:K:354:THR:HG23	1:K:354:THR:O	2.08	0.52
1:K:401:PRO:HA	1:K:404:LEU:HD12	1.91	0.52
1:D:71:GLU:HG2	1:D:92:SER:HB3	1.91	0.52
1:E:142:LEU:HG	1:E:252:LEU:HD11	1.92	0.52
1:I:24:VAL:HG12	1:I:109:PRO:HB3	1.91	0.52
1:J:133:MET:SD	1:J:150:PRO:HB2	2.50	0.52
1:J:199:SER:HB2	1:J:203:GLN:OE1	2.09	0.52
1:J:354:THR:CG2	1:J:381:TYR:OH	2.58	0.52
1:K:138:PHE:CG	1:K:191:VAL:HG11	2.45	0.52
1:K:142:LEU:HD12	1:K:248:ARG:CG	2.34	0.52
1:B:418:LEU:HD21	1:B:457:ALA:HA	1.91	0.52
1:E:219:GLU:OE1	1:E:283:GLN:CG	2.58	0.52
1:I:222:LEU:N	1:I:222:LEU:CD1	2.73	0.52
1:L:222:LEU:N	1:L:222:LEU:CD1	2.73	0.52
1:H:184:HIS:CE1	1:H:188:ARG:HG3	2.45	0.52
1:C:248:ARG:HH11	1:C:590:PRO:HA	1.74	0.52
1:E:315:LEU:HD22	1:F:319:PHE:HZ	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:80:GLU:O	1:G:83:VAL:HG22	2.10	0.52
1:G:180:LEU:HD11	1:G:221:LEU:HD21	1.91	0.52
1:K:547:LEU:H	1:K:547:LEU:HD12	1.74	0.52
1:L:165:ASN:HD21	1:L:523:GLN:HE22	1.58	0.52
1:A:41:LEU:HD13	1:A:66:VAL:HG12	1.91	0.52
1:B:566:ALA:HA	1:B:569:LEU:HD13	1.92	0.52
1:C:163:HIS:HB3	1:C:519:LEU:O	2.09	0.52
1:I:397:LEU:N	1:I:397:LEU:CD2	2.73	0.52
1:J:82:VAL:HG22	1:J:87:LEU:HD21	1.90	0.52
1:H:388:GLU:OE2	1:E:388:GLU:HG3	2.10	0.51
1:A:157:ASN:N	1:A:157:ASN:OD1	2.42	0.51
1:D:548:ALA:HB2	1:E:556:ARG:HB2	1.92	0.51
1:F:327:LYS:HE3	1:F:394:LYS:O	2.10	0.51
1:J:469:VAL:O	1:J:473:LYS:HG2	2.10	0.51
1:K:70:HIS:HB3	1:K:73:VAL:CG2	2.40	0.51
1:L:347:TRP:CG	1:L:347:TRP:O	2.58	0.51
1:L:372:PHE:O	1:L:376:ILE:HG13	2.10	0.51
1:H:70:HIS:ND1	1:H:73:VAL:HG21	2.25	0.51
1:H:263:GLN:HE21	1:H:265:LEU:HD21	1.75	0.51
1:H:315:LEU:HD22	1:L:319:PHE:CZ	2.40	0.51
1:E:249:TYR:OH	1:E:591:PHE:O	2.20	0.51
1:I:397:LEU:HB3	1:K:401:PRO:CG	2.37	0.51
1:J:453:LEU:HB3	1:J:457:ALA:HB3	1.92	0.51
1:K:249:TYR:O	1:K:254:LEU:O	2.28	0.51
1:F:57:VAL:HG13	1:F:104:PRO:HD2	1.91	0.51
1:K:219:GLU:HB3	1:K:283:GLN:HG3	1.92	0.51
1:K:502:LYS:HE3	1:K:530:GLU:HB2	1.91	0.51
1:H:219:GLU:OE1	1:H:283:GLN:HB2	2.11	0.51
1:H:219:GLU:OE2	1:H:283:GLN:HB2	2.10	0.51
1:B:149:LEU:HD13	1:B:585:VAL:HG21	1.93	0.51
1:D:530:GLU:OE2	1:D:532:ARG:HD3	2.10	0.51
1:I:588:ASN:ND2	1:I:588:ASN:H	2.05	0.51
1:J:87:LEU:CD1	1:J:87:LEU:N	2.72	0.51
1:J:547:LEU:H	1:J:547:LEU:HD12	1.76	0.51
1:L:159:GLU:OE1	1:L:203:GLN:NE2	2.43	0.51
1:H:24:VAL:O	1:H:109:PRO:HB3	2.10	0.51
1:B:223:PHE:N	1:B:284:ARG:HH11	2.08	0.51
1:D:155:PHE:CE1	1:D:160:SER:HB3	2.46	0.51
1:E:174:THR:HG21	3:E:1001:ADP:C4	2.45	0.51
1:G:560:GLN:HA	1:G:563:ARG:HG3	1.93	0.51
1:J:213:ILE:HG12	1:J:221:LEU:HD12	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:218:GLY:CA	1:J:451:HIS:HB2	2.40	0.51
1:K:294:THR:OG1	1:K:297:GLU:HG2	2.11	0.51
1:L:396:VAL:HG12	1:L:404:LEU:HD11	1.92	0.51
1:E:188:ARG:HH22	1:E:260:ARG:H	1.58	0.51
1:E:209:GLY:HA2	1:E:481:THR:O	2.11	0.51
1:F:158:GLY:HA2	1:F:161:GLY:O	2.10	0.51
1:F:226:LYS:CB	1:F:601:VAL:HG23	2.41	0.51
1:G:175:LYS:NZ	1:G:524:GLN:HA	2.24	0.51
1:A:190:GLY:O	1:A:193:ASP:HB2	2.11	0.51
1:A:570:GLN:HG3	1:A:571:PRO:HD2	1.93	0.51
1:B:223:PHE:HA	1:B:284:ARG:HH12	1.72	0.51
1:C:248:ARG:HH11	1:C:589:TYR:C	2.19	0.51
1:E:406:ALA:HA	1:E:409:ARG:HG2	1.92	0.51
1:J:579:PRO:HB3	1:L:172:VAL:HG21	1.93	0.51
1:B:396:VAL:O	1:B:399:GLN:HB2	2.11	0.51
1:D:153:PHE:CD2	1:D:195:THR:HG21	2.46	0.51
1:E:174:THR:HG22	3:E:1001:ADP:H5'2	1.93	0.51
1:K:278:VAL:HG23	1:K:278:VAL:O	2.10	0.51
1:A:41:LEU:HB2	1:B:107:PHE:HB3	1.93	0.51
1:B:500:PRO:O	1:B:503:ASP:HB2	2.11	0.51
1:C:60:TYR:HE1	1:C:103:ASP:HB2	1.76	0.51
1:E:175:LYS:N	3:E:1001:ADP:O1B	2.44	0.51
1:G:269:ARG:HA	1:G:280:GLN:HG2	1.91	0.51
1:L:62:LEU:O	1:L:98:LEU:N	2.38	0.51
1:L:238:VAL:HG11	1:L:248:ARG:NH2	2.22	0.51
1:H:242:LYS:HZ2	1:H:588:ASN:ND2	2.04	0.51
1:B:75:PHE:HD1	1:C:71:GLU:CG	2.23	0.51
1:E:199:SER:HB2	1:E:202:ARG:HG2	1.93	0.51
1:G:375:LEU:O	1:G:379:LEU:HG	2.10	0.51
1:I:173:ALA:HB2	1:I:544:ARG:N	2.26	0.51
1:J:156:ILE:HD13	1:J:164:ILE:HD11	1.92	0.51
1:J:401:PRO:HB2	1:K:397:LEU:CB	2.38	0.51
1:K:251:LEU:HD12	1:K:251:LEU:H	1.76	0.51
1:H:19:LEU:HD12	1:G:79:VAL:HG21	1.93	0.50
1:A:21:THR:HG21	1:F:76:GLU:HA	1.92	0.50
1:C:376:ILE:HD13	1:C:411:LEU:HB3	1.92	0.50
1:J:323:ASN:CG	1:L:405:ARG:HD2	2.36	0.50
1:H:248:ARG:HB2	1:H:590:PRO:HG3	1.92	0.50
1:H:291:PHE:HA	1:H:434:TYR:O	2.12	0.50
1:H:506:LEU:HD13	1:H:532:ARG:NH2	2.27	0.50
1:B:76:GLU:N	1:B:76:GLU:OE2	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:219:GLU:CD	1:E:283:GLN:HB2	2.36	0.50
1:E:386:GLU:HG3	1:E:387:ARG:HG3	1.93	0.50
1:J:269:ARG:HB2	1:J:278:VAL:HG23	1.94	0.50
1:J:324:ILE:HD12	1:J:407:PHE:CE2	2.41	0.50
1:K:199:SER:HB2	1:K:202:ARG:HB2	1.91	0.50
1:K:352:SER:O	1:K:352:SER:OG	2.30	0.50
1:B:478:ARG:HG3	1:B:516:GLY:CA	2.38	0.50
1:C:263:GLN:HE21	1:C:265:LEU:HD21	1.76	0.50
1:C:453:LEU:HB3	1:C:457:ALA:HB3	1.93	0.50
1:G:155:PHE:C	1:G:161:GLY:HA3	2.35	0.50
1:G:264:LEU:HD23	1:G:447:VAL:HB	1.93	0.50
1:G:319:PHE:HZ	1:I:315:LEU:HD21	1.77	0.50
1:L:219:GLU:OE2	1:L:282:ASP:OD1	2.28	0.50
1:H:71:GLU:OE2	1:G:76:GLU:N	2.45	0.50
1:H:131:ASP:OD1	1:H:131:ASP:N	2.39	0.50
1:B:195:THR:HG23	1:B:203:GLN:HE22	1.76	0.50
1:C:473:LYS:HG3	1:C:517:ILE:HG12	1.93	0.50
1:D:397:LEU:O	1:D:398:LYS:HE3	2.12	0.50
1:E:174:THR:OG1	1:E:589:TYR:OH	2.04	0.50
1:E:249:TYR:HE1	1:E:590:PRO:HB2	1.73	0.50
1:F:184:HIS:CE1	1:F:188:ARG:HG3	2.46	0.50
1:K:153:PHE:CE2	1:K:157:ASN:HB3	2.46	0.50
1:A:597:ARG:NH2	1:A:599:ASP:OD2	2.45	0.50
1:B:103:ASP:CB	1:B:104:PRO:HD3	2.40	0.50
1:C:371:THR:OG1	1:C:373:GLU:OE1	2.30	0.50
1:F:386:GLU:HG3	1:F:387:ARG:HG3	1.92	0.50
1:I:52:PRO:HD2	1:K:38:SER:HB3	1.93	0.50
1:I:184:HIS:CE1	1:I:188:ARG:HG3	2.46	0.50
1:L:181:PHE:CE1	1:L:590:PRO:HD2	2.46	0.50
1:H:109:PRO:HG3	1:G:66:VAL:HG13	1.94	0.50
1:B:155:PHE:CD1	1:B:579:PRO:HG2	2.46	0.50
1:B:324:ILE:N	1:B:324:ILE:CD1	2.74	0.50
1:C:400:SER:HB2	1:D:398:LYS:HZ2	1.75	0.50
1:D:76:GLU:N	1:E:71:GLU:OE2	2.35	0.50
1:D:385:GLU:HA	1:D:389:GLY:HA2	1.93	0.50
1:F:352:SER:HB3	1:F:385:GLU:OE2	2.11	0.50
1:I:478:ARG:HG2	1:I:478:ARG:O	2.11	0.50
1:L:386:GLU:HG3	1:L:387:ARG:HG3	1.92	0.50
1:A:268:PRO:HG3	1:A:292:VAL:HG12	1.93	0.50
1:A:349:PHE:HB2	1:A:354:THR:HB	1.93	0.50
1:B:42:ASP:OD2	1:B:586:LEU:HD22	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:560:GLN:HG2	1:E:563:ARG:NH1	2.26	0.50
1:G:315:LEU:HD23	1:G:317:LEU:HD11	1.93	0.50
1:I:33:VAL:HG21	1:I:93:TYR:CD2	2.46	0.50
1:J:184:HIS:CE1	1:J:188:ARG:HG3	2.47	0.50
1:J:560:GLN:HG2	1:J:563:ARG:NH1	2.26	0.50
1:K:513:ARG:NH1	1:K:513:ARG:CB	2.73	0.50
1:L:344:VAL:HG23	1:L:344:VAL:O	2.11	0.50
1:A:135:GLU:OE2	1:A:154:ARG:NH2	2.45	0.50
1:A:560:GLN:HA	1:A:563:ARG:HG3	1.93	0.50
1:B:470:PHE:HD1	1:B:517:ILE:HD12	1.76	0.50
1:C:315:LEU:HD23	1:C:317:LEU:HD12	1.93	0.50
1:D:236:ASP:O	1:D:240:ARG:HG2	2.12	0.50
1:J:40:GLY:N	1:J:43:ASP:OD2	2.45	0.50
1:L:51:LYS:N	1:L:55:THR:O	2.35	0.50
1:L:473:LYS:HB3	1:L:515:LEU:HG	1.94	0.50
1:C:406:ALA:HA	1:C:409:ARG:HG2	1.94	0.50
1:D:221:LEU:HD22	1:D:224:LEU:HD11	1.94	0.50
1:D:381:TYR:CZ	1:D:386:GLU:OE2	2.65	0.50
1:E:202:ARG:HG3	1:E:203:GLN:N	2.27	0.50
1:F:102:VAL:HB	1:F:105:GLU:HA	1.94	0.50
1:I:19:LEU:HD13	1:I:32:ALA:HB2	1.93	0.50
1:J:143:LEU:HB3	1:J:587:VAL:HG12	1.93	0.50
1:K:181:PHE:CE1	1:K:590:PRO:HD2	2.47	0.50
1:K:266:ALA:HB1	1:K:267:PRO:HD2	1.93	0.50
1:H:193:ASP:OD1	1:H:206:THR:HG22	2.11	0.49
1:H:405:ARG:HD3	1:L:323:ASN:HA	1.94	0.49
1:B:57:VAL:HG13	1:B:104:PRO:HD2	1.94	0.49
1:C:175:LYS:NZ	1:C:524:GLN:HA	2.27	0.49
1:D:310:ASP:OD2	1:D:314:SER:HB3	2.12	0.49
1:E:41:LEU:HD13	1:E:66:VAL:HG12	1.92	0.49
1:E:82:VAL:HG13	1:E:89:ALA:HB2	1.93	0.49
1:F:242:LYS:HB2	1:F:244:LEU:CD1	2.41	0.49
1:G:162:GLY:O	1:G:518:ILE:HD12	2.12	0.49
1:J:310:ASP:CG	1:J:314:SER:HB3	2.37	0.49
1:K:44:LEU:HD21	1:K:62:LEU:HD12	1.94	0.49
1:K:174:THR:OG1	1:K:589:TYR:OH	2.15	0.49
1:H:383:LEU:HG	1:H:404:LEU:HD22	1.93	0.49
1:C:175:LYS:NZ	1:C:523:GLN:C	2.70	0.49
1:E:156:ILE:HD13	1:E:164:ILE:HD11	1.95	0.49
1:G:371:THR:OG1	1:G:373:GLU:OE1	2.30	0.49
1:I:269:ARG:O	1:I:269:ARG:HG3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:25:THR:HG23	1:L:26:PRO:HD2	1.93	0.49
1:L:410:ARG:HH22	1:L:456:HIS:CD2	2.30	0.49
1:L:478:ARG:O	1:L:478:ARG:HD3	2.12	0.49
1:A:142:LEU:CD1	1:A:248:ARG:HB3	2.41	0.49
1:A:143:LEU:C	1:A:143:LEU:CD1	2.85	0.49
1:B:553:PRO:HA	1:B:556:ARG:HD3	1.92	0.49
1:C:79:VAL:HG21	1:D:19:LEU:HD12	1.93	0.49
1:D:320:VAL:CG2	1:D:399:GLN:HG2	2.41	0.49
1:D:478:ARG:HG3	1:D:515:LEU:C	2.37	0.49
1:F:80:GLU:OE2	1:F:80:GLU:HA	2.11	0.49
1:G:128:LEU:HD13	1:G:150:PRO:HD2	1.95	0.49
1:J:149:LEU:HD22	1:J:587:VAL:HG11	1.94	0.49
1:L:326:GLU:HG3	1:L:330:ARG:NH1	2.28	0.49
1:B:223:PHE:HE1	1:B:284:ARG:HB2	1.75	0.49
1:B:376:ILE:HD13	1:B:411:LEU:HB3	1.95	0.49
1:E:315:LEU:HG	1:E:316:ASN:N	2.27	0.49
1:I:33:VAL:CG2	1:I:93:TYR:CD2	2.95	0.49
1:J:26:PRO:O	1:J:99:VAL:HG21	2.11	0.49
1:J:349:PHE:HB2	1:J:352:SER:CB	2.24	0.49
1:L:75:PHE:HB3	1:L:78:ASP:HB2	1.94	0.49
1:L:248:ARG:HH11	1:L:589:TYR:C	2.20	0.49
1:H:315:LEU:HG	1:H:316:ASN:H	1.78	0.49
1:I:59:PHE:CD1	1:I:110:PRO:HG3	2.47	0.49
1:I:133:MET:SD	1:I:150:PRO:HB2	2.53	0.49
1:J:473:LYS:NZ	1:J:480:ASP:O	2.34	0.49
1:K:188:ARG:CG	1:K:188:ARG:NH1	2.73	0.49
1:K:499:SER:HB2	1:K:500:PRO:CD	2.43	0.49
1:L:50:ARG:HA	1:L:56:PRO:HA	1.94	0.49
1:H:466:LEU:HD21	1:H:484:VAL:HG11	1.95	0.49
1:A:320:VAL:HG21	1:A:403:THR:HG22	1.93	0.49
1:B:175:LYS:NZ	1:B:524:GLN:HA	2.27	0.49
1:C:57:VAL:HG13	1:C:104:PRO:HD2	1.94	0.49
1:E:470:PHE:CZ	1:E:507:ASP:HB3	2.48	0.49
1:G:149:LEU:HD21	1:G:576:VAL:HG21	1.94	0.49
1:I:158:GLY:HA2	1:I:513:ARG:HB3	1.94	0.49
1:J:87:LEU:HD22	1:J:87:LEU:C	2.38	0.49
1:L:31:PHE:CE1	1:L:33:VAL:HG12	2.47	0.49
1:L:84:ALA:HB3	1:L:86:LEU:HD23	1.93	0.49
1:A:347:TRP:CH2	1:A:354:THR:HG21	2.47	0.49
1:B:75:PHE:CE1	1:C:71:GLU:HG3	2.47	0.49
1:B:80:GLU:H	1:B:80:GLU:CD	2.16	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:248:ARG:HH11	1:B:590:PRO:HA	1.77	0.49
1:E:143:LEU:C	1:E:143:LEU:CD1	2.85	0.49
1:F:174:THR:HG22	3:F:1001:ADP:H5'2	1.94	0.49
1:I:291:PHE:C	1:I:291:PHE:CD2	2.90	0.49
1:I:553:PRO:HA	1:I:556:ARG:HD3	1.94	0.49
1:A:143:LEU:HD12	1:A:143:LEU:O	2.12	0.49
1:B:174:THR:CB	3:B:1001:ADP:H5'2	2.43	0.49
1:C:238:VAL:HG11	1:C:248:ARG:NH2	2.18	0.49
1:D:175:LYS:NZ	1:D:523:GLN:C	2.70	0.49
1:J:219:GLU:OE1	1:J:283:GLN:CB	2.46	0.49
1:K:175:LYS:HZ3	1:K:524:GLN:HA	1.78	0.49
1:K:428:PRO:HA	1:K:431:ALA:HB3	1.95	0.49
1:D:263:GLN:HB2	1:D:443:ILE:CG2	2.42	0.49
1:F:64:ASP:OD1	1:F:96:ARG:HD2	2.13	0.49
1:L:248:ARG:HB2	1:L:590:PRO:HG3	1.94	0.49
1:A:228:ASN:HD22	1:A:600:GLU:HB3	1.77	0.49
1:D:41:LEU:HD13	1:D:66:VAL:HG12	1.94	0.49
1:G:376:ILE:HD13	1:G:411:LEU:HB3	1.94	0.49
1:J:68:LYS:HD3	1:K:111:GLN:HG2	1.94	0.49
1:L:323:ASN:HD21	1:L:397:LEU:HD13	1.78	0.49
1:B:153:PHE:HD2	1:B:195:THR:HG21	1.78	0.48
1:D:231:MET:HE3	1:D:232:VAL:HG13	1.94	0.48
1:E:66:VAL:HG13	1:F:109:PRO:HG3	1.94	0.48
1:E:174:THR:CA	3:E:1001:ADP:H5'2	2.42	0.48
1:K:142:LEU:CD1	1:K:248:ARG:HG2	2.35	0.48
1:K:297:GLU:OE1	1:K:301:ARG:CD	2.60	0.48
1:K:481:THR:O	1:K:481:THR:OG1	2.30	0.48
1:H:189:SER:O	1:H:194:ARG:NH2	2.41	0.48
1:A:131:ASP:OD1	1:A:131:ASP:N	2.40	0.48
1:E:343:ILE:HA	1:E:367:VAL:O	2.13	0.48
1:J:380:GLU:O	1:J:384:LEU:HB2	2.12	0.48
1:K:155:PHE:HA	1:K:161:GLY:CA	2.38	0.48
1:L:60:TYR:CE1	1:L:103:ASP:HB2	2.44	0.48
1:L:166:ILE:HG23	1:L:541:VAL:HB	1.94	0.48
1:H:183:LEU:HD22	1:H:187:PHE:CE2	2.48	0.48
1:H:556:ARG:HB2	1:G:548:ALA:CB	2.43	0.48
1:A:174:THR:HG22	3:A:1001:ADP:C5'	2.37	0.48
1:C:104:PRO:HD2	1:C:104:PRO:O	2.12	0.48
1:D:238:VAL:HG11	1:D:248:ARG:NH2	2.29	0.48
1:G:291:PHE:HB2	1:G:436:PRO:HG3	1.94	0.48
1:J:158:GLY:HA2	1:J:161:GLY:O	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:199:SER:OG	1:L:597:ARG:HD3	2.13	0.48
1:J:530:GLU:OE2	1:J:532:ARG:HD3	2.13	0.48
1:K:220:ASP:HA	1:K:596:THR:O	2.13	0.48
1:K:269:ARG:O	1:K:269:ARG:CG	2.47	0.48
1:L:176:THR:OG1	1:L:487:ASP:OD2	2.30	0.48
1:A:221:LEU:HD22	1:A:224:LEU:HD11	1.95	0.48
1:A:236:ASP:O	1:A:240:ARG:HG2	2.13	0.48
1:B:175:LYS:HZ3	1:B:524:GLN:HA	1.78	0.48
1:C:353:GLU:OE2	1:C:353:GLU:HA	2.13	0.48
1:I:47:VAL:HG13	1:I:59:PHE:HB2	1.95	0.48
1:C:231:MET:SD	1:C:249:TYR:CE2	3.07	0.48
1:C:362:SER:N	1:C:366:GLY:O	2.34	0.48
1:E:40:GLY:N	1:E:43:ASP:OD2	2.44	0.48
1:F:376:ILE:HD13	1:F:411:LEU:HB3	1.94	0.48
1:I:418:LEU:HD21	1:I:457:ALA:HA	1.95	0.48
1:J:386:GLU:OE1	1:J:392:ASP:HB2	2.14	0.48
1:K:136:ALA:HA	1:K:195:THR:HG21	1.95	0.48
1:K:473:LYS:HB2	1:K:517:ILE:HD11	1.94	0.48
1:L:33:VAL:HG22	1:L:93:TYR:O	2.13	0.48
1:B:219:GLU:HB3	1:B:222:LEU:CD1	2.44	0.48
1:D:219:GLU:OE1	1:D:283:GLN:NE2	2.47	0.48
1:D:553:PRO:HA	1:D:556:ARG:HD3	1.96	0.48
1:F:165:ASN:ND2	1:F:523:GLN:HE22	2.08	0.48
1:F:199:SER:HB3	1:F:203:GLN:H	1.78	0.48
1:L:349:PHE:O	1:L:349:PHE:CD1	2.67	0.48
1:A:157:ASN:ND2	1:A:159:GLU:HG3	2.29	0.48
1:B:294:THR:HB	1:B:340:THR:HB	1.96	0.48
1:B:570:GLN:HG3	1:B:571:PRO:HD2	1.95	0.48
1:C:268:PRO:HG3	1:C:292:VAL:HG12	1.94	0.48
1:C:387:ARG:C	1:C:388:GLU:OE1	2.56	0.48
1:G:40:GLY:N	1:G:43:ASP:OD2	2.46	0.48
1:I:24:VAL:O	1:K:67:ARG:HA	2.14	0.48
1:I:478:ARG:HG3	1:I:516:GLY:CA	2.43	0.48
1:K:184:HIS:C	1:K:184:HIS:CD2	2.92	0.48
1:L:357:GLU:OE1	1:L:358:ASN:O	2.31	0.48
1:L:423:ARG:NH1	1:L:426:LEU:HD21	2.29	0.48
1:H:175:LYS:HD2	1:H:522:ALA:HB1	1.95	0.48
1:B:149:LEU:HD21	1:B:576:VAL:HG21	1.94	0.48
1:B:353:GLU:HG3	1:B:353:GLU:O	2.13	0.48
1:C:199:SER:HB2	1:C:203:GLN:H	1.79	0.48
1:D:51:LYS:HG2	1:D:52:PRO:HD2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:149:LEU:HD21	1:D:576:VAL:HG21	1.95	0.48
1:I:142:LEU:O	1:I:588:ASN:N	2.43	0.48
1:L:24:VAL:HG11	1:L:110:PRO:O	2.13	0.48
1:L:64:ASP:OD1	1:L:96:ARG:HD2	2.14	0.48
1:H:195:THR:C	1:H:203:GLN:NE2	2.72	0.48
1:A:386:GLU:HG3	1:A:387:ARG:HG3	1.95	0.48
1:D:397:LEU:C	1:D:398:LYS:HG3	2.39	0.48
1:D:441:ARG:CG	1:D:441:ARG:NH2	2.73	0.48
1:E:335:GLN:CD	1:E:343:ILE:H	2.22	0.48
1:F:19:LEU:HD13	1:F:32:ALA:HB2	1.95	0.48
1:I:268:PRO:HD2	1:I:421:LEU:HD23	1.96	0.48
1:K:165:ASN:OD1	1:K:523:GLN:NE2	2.37	0.48
1:L:587:VAL:C	1:L:588:ASN:HD22	2.22	0.48
1:H:553:PRO:HA	1:H:556:ARG:HD3	1.94	0.48
1:A:376:ILE:HD13	1:A:411:LEU:HB3	1.95	0.48
1:A:402:GLY:C	1:B:319:PHE:CE1	2.92	0.48
1:B:76:GLU:CD	1:B:76:GLU:H	2.20	0.48
1:G:228:ASN:CG	1:G:600:GLU:OE2	2.57	0.48
1:J:379:LEU:CD2	1:J:395:TRP:HZ3	2.27	0.48
1:H:386:GLU:HB3	1:H:392:ASP:N	2.29	0.47
1:H:530:GLU:HG3	1:H:532:ARG:H	1.79	0.47
1:H:597:ARG:CG	1:H:600:GLU:HG3	2.44	0.47
1:C:553:PRO:O	1:C:556:ARG:HG2	2.14	0.47
1:F:153:PHE:CD2	1:F:195:THR:HG21	2.48	0.47
1:H:453:LEU:HB3	1:H:457:ALA:HB3	1.96	0.47
1:A:406:ALA:HA	1:A:409:ARG:HG2	1.95	0.47
1:B:525:THR:HG22	1:B:527:SER:H	1.79	0.47
1:E:64:ASP:OD1	1:E:96:ARG:HD2	2.14	0.47
1:E:274:GLY:O	1:E:423:ARG:NH2	2.45	0.47
1:G:149:LEU:HD22	1:G:587:VAL:HG11	1.95	0.47
1:J:192:MET:HE1	1:J:209:GLY:HA3	1.96	0.47
1:L:149:LEU:HD21	1:L:576:VAL:HG21	1.96	0.47
1:H:64:ASP:OD1	1:H:96:ARG:HD2	2.14	0.47
1:H:175:LYS:N	3:H:1001:ADP:O3B	2.46	0.47
1:H:550:ALA:HB1	1:H:563:ARG:HB3	1.96	0.47
1:B:213:ILE:CD1	1:B:221:LEU:CD1	2.92	0.47
1:J:299:CYS:HB2	1:J:332:ALA:HB2	1.96	0.47
1:K:213:ILE:CG2	1:K:447:VAL:HG22	2.44	0.47
1:K:269:ARG:HB2	1:K:278:VAL:HG23	1.96	0.47
1:K:387:ARG:C	1:K:388:GLU:HG2	2.40	0.47
1:H:166:ILE:HG22	1:H:175:LYS:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:215:ASN:HD21	1:H:219:GLU:H	1.62	0.47
1:H:242:LYS:HZ3	1:H:588:ASN:HD21	1.60	0.47
1:B:219:GLU:CB	1:B:222:LEU:CD1	2.92	0.47
1:B:268:PRO:HD3	1:B:291:PHE:O	2.14	0.47
1:B:525:THR:HG21	1:B:549:GLU:OE1	2.14	0.47
1:D:248:ARG:HB2	1:D:590:PRO:HG3	1.96	0.47
1:E:36:GLY:HA2	1:F:52:PRO:HB3	1.96	0.47
1:E:41:LEU:HB2	1:F:107:PHE:CB	2.45	0.47
1:L:101:ARG:HH12	1:L:131:ASP:CG	2.22	0.47
1:L:242:LYS:NZ	1:L:588:ASN:OD1	2.47	0.47
1:H:597:ARG:HG2	1:H:600:GLU:HG3	1.95	0.47
1:C:149:LEU:HD21	1:C:576:VAL:HG21	1.96	0.47
1:E:211:ALA:HA	1:E:483:PHE:O	2.13	0.47
1:G:52:PRO:HD2	1:I:38:SER:HB3	1.97	0.47
1:J:354:THR:HG23	1:J:381:TYR:CE2	2.46	0.47
1:J:599:ASP:OD1	1:J:599:ASP:N	2.47	0.47
1:L:49:THR:HG21	1:L:110:PRO:HA	1.97	0.47
1:L:84:ALA:CB	1:L:86:LEU:CD2	2.92	0.47
1:A:175:LYS:HZ3	1:A:524:GLN:HA	1.80	0.47
1:A:215:ASN:HB3	1:A:449:ASP:HA	1.96	0.47
1:B:75:PHE:HD1	1:C:71:GLU:HG2	1.79	0.47
1:C:162:GLY:H	1:C:538:ALA:HB2	1.79	0.47
1:C:191:VAL:O	1:C:195:THR:HG22	2.15	0.47
1:C:320:VAL:HG22	1:C:399:GLN:HG2	1.96	0.47
1:J:175:LYS:NZ	1:J:524:GLN:HA	2.30	0.47
1:H:70:HIS:CG	1:H:73:VAL:HG21	2.50	0.47
1:H:269:ARG:HA	1:H:280:GLN:HG2	1.97	0.47
1:A:19:LEU:HD13	1:A:32:ALA:HB2	1.96	0.47
1:A:228:ASN:ND2	1:A:600:GLU:OE1	2.48	0.47
1:B:190:GLY:O	1:B:193:ASP:HB2	2.14	0.47
1:B:191:VAL:O	1:B:195:THR:HG22	2.14	0.47
1:B:473:LYS:CG	1:B:517:ILE:HD11	2.43	0.47
1:C:69:ARG:NE	1:D:23:ASP:OD1	2.42	0.47
1:D:281:THR:OG1	1:D:284:ARG:O	2.19	0.47
1:E:169:ILE:HG22	1:E:172:VAL:HB	1.97	0.47
1:F:474:GLU:OE1	1:F:511:ARG:NH2	2.47	0.47
1:I:223:PHE:HB3	1:I:601:VAL:HG21	1.96	0.47
1:I:323:ASN:ND2	1:I:397:LEU:HD23	2.30	0.47
1:J:61:GLY:HA2	1:J:100:THR:H	1.80	0.47
1:J:64:ASP:OD1	1:J:96:ARG:HD2	2.15	0.47
1:J:324:ILE:HD12	1:J:407:PHE:CE1	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:294:THR:HB	1:K:340:THR:HB	1.95	0.47
1:L:326:GLU:CG	1:L:330:ARG:NH1	2.78	0.47
1:L:423:ARG:NH1	1:L:425:ASP:OD1	2.47	0.47
1:A:108:ILE:O	1:A:108:ILE:HG13	2.14	0.47
1:A:193:ASP:CG	1:A:206:THR:HG21	2.40	0.47
1:C:40:GLY:N	1:C:43:ASP:OD2	2.47	0.47
1:C:175:LYS:HD2	1:C:522:ALA:HB1	1.95	0.47
1:E:41:LEU:HB2	1:F:107:PHE:HB2	1.96	0.47
1:E:58:ARG:HB2	1:E:103:ASP:HB3	1.97	0.47
1:E:155:PHE:HD1	1:E:161:GLY:HA3	1.80	0.47
1:G:553:PRO:HA	1:G:556:ARG:HD3	1.96	0.47
1:K:502:LYS:HG2	1:K:506:LEU:CD1	2.44	0.47
1:L:268:PRO:HG3	1:L:292:VAL:HG12	1.95	0.47
1:H:373:GLU:HA	1:H:415:GLN:OE1	2.14	0.47
1:A:149:LEU:HD22	1:A:587:VAL:CG1	2.42	0.47
1:A:349:PHE:CE1	1:A:356:PRO:CG	2.92	0.47
1:B:64:ASP:OD1	1:B:96:ARG:HD2	2.15	0.47
1:D:553:PRO:O	1:D:556:ARG:HG2	2.15	0.47
1:E:282:ASP:OD1	1:E:282:ASP:N	2.40	0.47
1:I:363:GLU:H	1:I:363:GLU:CD	2.22	0.47
1:J:142:LEU:HA	1:J:142:LEU:HD23	1.75	0.47
1:K:149:LEU:HD21	1:K:576:VAL:HG21	1.97	0.47
1:K:248:ARG:O	1:K:251:LEU:N	2.48	0.47
1:H:291:PHE:HD2	1:H:436:PRO:HG3	1.80	0.47
1:A:249:TYR:OH	1:A:591:PHE:O	2.27	0.47
1:C:165:ASN:HD21	1:C:523:GLN:NE2	2.11	0.47
1:C:189:SER:O	1:C:194:ARG:NH2	2.48	0.47
1:D:162:GLY:CA	1:D:538:ALA:HB2	2.43	0.47
1:D:173:ALA:HB1	1:D:543:GLY:HA3	1.97	0.47
1:E:70:HIS:HB2	1:F:20:GLY:HA3	1.97	0.47
1:F:191:VAL:O	1:F:195:THR:HG22	2.14	0.47
1:F:284:ARG:O	1:F:288:VAL:HG21	2.15	0.47
1:I:174:THR:HG1	1:I:589:TYR:HH	1.62	0.47
1:J:63:VAL:HA	1:J:96:ARG:O	2.15	0.47
1:K:502:LYS:HG2	1:K:506:LEU:HD11	1.96	0.47
1:L:51:LYS:HG3	1:L:57:VAL:HG21	1.97	0.47
1:H:228:ASN:ND2	1:H:600:GLU:OE1	2.48	0.46
1:D:469:VAL:O	1:D:473:LYS:HG2	2.15	0.46
1:F:248:ARG:HD2	1:F:590:PRO:HA	1.97	0.46
1:K:215:ASN:ND2	1:K:215:ASN:C	2.72	0.46
1:H:17:MET:HE1	1:G:83:VAL:HG11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:506:LEU:HD23	1:H:533:ILE:HD12	1.97	0.46
1:A:299:CYS:HB2	1:A:332:ALA:HB2	1.98	0.46
1:D:87:LEU:C	1:D:87:LEU:CD2	2.86	0.46
1:F:133:MET:HG2	1:F:152:ASN:HB2	1.97	0.46
1:F:248:ARG:HH11	1:F:590:PRO:HA	1.81	0.46
1:G:153:PHE:HD2	1:G:195:THR:HG21	1.80	0.46
1:I:159:GLU:OE1	1:I:203:GLN:NE2	2.48	0.46
1:I:339:GLY:HA2	1:I:428:PRO:HG3	1.97	0.46
1:J:191:VAL:O	1:J:195:THR:HG22	2.15	0.46
1:K:131:ASP:OD1	1:K:131:ASP:N	2.48	0.46
1:K:139:PRO:HG2	1:K:254:LEU:HD21	1.95	0.46
1:K:153:PHE:HE1	1:K:186:ILE:HD13	1.79	0.46
1:L:64:ASP:OD1	1:L:65:ASN:N	2.49	0.46
1:A:146:GLY:CA	1:A:251:LEU:HD23	2.42	0.46
1:B:171:GLY:N	3:B:1001:ADP:O2B	2.37	0.46
1:B:291:PHE:HA	1:B:434:TYR:O	2.15	0.46
1:D:291:PHE:HA	1:D:434:TYR:O	2.15	0.46
1:D:566:ALA:HA	1:D:569:LEU:CG	2.42	0.46
1:G:387:ARG:O	1:G:388:GLU:CG	2.62	0.46
1:H:269:ARG:HB2	1:H:278:VAL:HG23	1.96	0.46
1:H:478:ARG:HD2	1:H:514:SER:O	2.15	0.46
1:B:80:GLU:OE2	1:B:80:GLU:N	2.40	0.46
1:B:173:ALA:HB1	1:B:543:GLY:HA3	1.97	0.46
1:C:248:ARG:NH1	1:C:590:PRO:HA	2.31	0.46
1:D:82:VAL:HG23	1:D:87:LEU:HD22	1.87	0.46
1:E:387:ARG:O	1:E:390:GLU:HG2	2.16	0.46
1:F:176:THR:HB	3:F:1001:ADP:O2A	2.15	0.46
1:I:513:ARG:HH22	1:K:217:LYS:HE2	1.80	0.46
1:K:231:MET:SD	1:K:249:TYR:HE2	2.39	0.46
1:H:291:PHE:HB2	1:H:436:PRO:HG3	1.97	0.46
1:A:267:PRO:HG2	1:A:280:GLN:HG3	1.97	0.46
1:B:320:VAL:HG21	1:B:403:THR:HG22	1.98	0.46
1:E:133:MET:CG	1:E:152:ASN:HB2	2.46	0.46
1:F:155:PHE:CD1	1:F:579:PRO:HG2	2.51	0.46
1:K:64:ASP:OD1	1:K:96:ARG:HD2	2.15	0.46
1:K:298:PHE:CD2	1:K:422:ILE:HD13	2.51	0.46
1:K:426:LEU:N	1:K:426:LEU:HD23	2.30	0.46
1:K:514:SER:OG	1:K:515:LEU:HD12	2.16	0.46
1:L:406:ALA:HA	1:L:409:ARG:HG2	1.96	0.46
1:L:495:ARG:NE	1:L:527:SER:O	2.48	0.46
1:H:216:VAL:HG11	1:H:488:GLU:OE1	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:ARG:HB2	1:A:482:VAL:HG22	1.98	0.46
1:B:223:PHE:CA	1:B:284:ARG:NH1	2.70	0.46
1:F:228:ASN:OD1	1:F:600:GLU:HB3	2.16	0.46
1:G:71:GLU:OE2	1:I:76:GLU:N	2.45	0.46
1:G:176:THR:OG1	1:G:487:ASP:OD2	2.33	0.46
1:J:597:ARG:CG	1:J:600:GLU:HG3	2.45	0.46
1:K:196:ALA:HB1	1:K:205:GLY:HA2	1.97	0.46
1:K:436:PRO:O	1:K:436:PRO:HG2	2.15	0.46
1:K:553:PRO:HA	1:K:556:ARG:HD3	1.98	0.46
1:H:501:ILE:O	1:H:504:VAL:HG12	2.16	0.46
1:C:73:VAL:HG12	1:C:82:VAL:HG21	1.98	0.46
1:C:473:LYS:HG3	1:C:517:ILE:CG1	2.45	0.46
1:D:161:GLY:HA2	1:D:513:ARG:HH21	1.76	0.46
1:E:101:ARG:NH2	1:E:131:ASP:OD1	2.47	0.46
1:G:57:VAL:HA	1:G:104:PRO:HG2	1.98	0.46
1:I:40:GLY:O	1:I:63:VAL:HG11	2.15	0.46
1:L:19:LEU:N	1:L:31:PHE:HA	2.30	0.46
1:C:248:ARG:HB2	1:C:590:PRO:HG3	1.96	0.46
1:D:70:HIS:CB	1:D:73:VAL:CG2	2.80	0.46
1:E:101:ARG:HH22	1:E:131:ASP:CG	2.23	0.46
1:E:247:ASP:OD1	1:E:247:ASP:N	2.47	0.46
1:I:100:THR:HG22	1:I:583:ASN:ND2	2.31	0.46
1:L:421:LEU:HD11	1:L:453:LEU:HD11	1.98	0.46
1:B:219:GLU:C	1:B:222:LEU:HD12	2.41	0.46
1:B:223:PHE:CA	1:B:284:ARG:HH11	2.27	0.46
1:C:320:VAL:HG21	1:C:403:THR:HG22	1.98	0.46
1:C:525:THR:HG22	1:C:527:SER:H	1.81	0.46
1:E:268:PRO:HG3	1:E:292:VAL:HG12	1.97	0.46
1:G:335:GLN:NE2	1:G:343:ILE:O	2.46	0.46
1:I:231:MET:HE2	1:I:231:MET:HB3	1.78	0.46
1:J:591:PHE:CZ	3:J:1001:ADP:C2	3.04	0.46
1:K:79:VAL:O	1:K:83:VAL:HG13	2.16	0.46
1:H:231:MET:HE3	1:H:232:VAL:HG13	1.98	0.46
1:H:269:ARG:HB2	1:H:278:VAL:O	2.16	0.46
1:H:387:ARG:NH1	1:H:393:PRO:HD2	2.30	0.46
1:A:66:VAL:HG13	1:B:109:PRO:HG3	1.98	0.46
1:B:195:THR:HG23	1:B:203:GLN:NE2	2.31	0.46
1:C:41:LEU:HD13	1:C:66:VAL:HG12	1.97	0.46
1:C:165:ASN:ND2	1:C:523:GLN:HE22	2.10	0.46
1:F:355:PRO:N	1:F:355:PRO:C	2.65	0.46
1:L:560:GLN:HA	1:L:563:ARG:HG3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:228:ASN:ND2	1:B:600:GLU:HB3	2.31	0.45
1:C:242:LYS:HB2	1:C:244:LEU:CD1	2.43	0.45
1:D:41:LEU:HB2	1:E:107:PHE:CB	2.46	0.45
1:G:156:ILE:CD1	1:G:164:ILE:HD11	2.46	0.45
1:I:324:ILE:N	1:I:324:ILE:CD1	2.78	0.45
1:I:414:VAL:HG22	1:I:418:LEU:HG	1.97	0.45
1:K:215:ASN:CG	1:K:218:GLY:O	2.59	0.45
1:K:246:ALA:O	1:K:251:LEU:CD1	2.57	0.45
1:E:174:THR:HG21	3:E:1001:ADP:N9	2.32	0.45
1:E:335:GLN:NE2	1:E:343:ILE:H	2.14	0.45
1:I:248:ARG:HB3	1:I:590:PRO:HG3	1.99	0.45
1:L:191:VAL:O	1:L:195:THR:HG22	2.17	0.45
1:L:393:PRO:O	1:L:397:LEU:HD12	2.16	0.45
1:L:523:GLN:HG3	1:L:529:VAL:HG21	1.98	0.45
1:H:126:MET:HE3	1:H:126:MET:HB3	1.88	0.45
1:I:244:LEU:HD12	1:I:244:LEU:HA	1.76	0.45
1:K:281:THR:OG1	1:K:281:THR:O	2.34	0.45
1:K:386:GLU:HG3	1:K:387:ARG:HG3	1.99	0.45
1:H:331:LEU:HD21	1:H:344:VAL:HG12	1.98	0.45
1:A:80:GLU:H	1:A:80:GLU:HG2	1.58	0.45
1:F:51:LYS:HG2	1:F:52:PRO:HD2	1.98	0.45
1:F:284:ARG:HG2	1:F:288:VAL:CG2	2.47	0.45
1:I:370:GLN:HB3	1:I:425:ASP:HB3	1.98	0.45
1:I:566:ALA:HA	1:I:569:LEU:CG	2.44	0.45
1:J:78:ASP:O	1:J:82:VAL:HG23	2.16	0.45
1:K:372:PHE:CE1	1:K:422:ILE:HD12	2.51	0.45
1:A:335:GLN:HG3	1:A:342:LEU:HD12	1.98	0.45
1:C:175:LYS:N	3:C:1001:ADP:O1B	2.49	0.45
1:D:184:HIS:CE1	1:D:188:ARG:HG3	2.51	0.45
1:D:228:ASN:ND2	1:D:231:MET:N	2.64	0.45
1:D:269:ARG:HB2	1:D:278:VAL:HG23	1.99	0.45
1:E:473:LYS:HB3	1:E:515:LEU:HG	1.98	0.45
1:E:473:LYS:NZ	1:E:480:ASP:O	2.42	0.45
1:F:188:ARG:NH2	1:F:260:ARG:HG3	2.31	0.45
1:G:221:LEU:HD23	1:G:221:LEU:HA	1.82	0.45
1:G:386:GLU:HG3	1:G:387:ARG:HG3	1.99	0.45
1:J:64:ASP:OD1	1:J:65:ASN:N	2.49	0.45
1:J:375:LEU:O	1:J:379:LEU:HG	2.17	0.45
1:J:379:LEU:HD23	1:J:395:TRP:HZ3	1.82	0.45
1:K:62:LEU:HD23	1:K:63:VAL:O	2.17	0.45
1:K:419:SER:HB3	1:K:420:PRO:HD3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:248:ARG:NH1	1:L:589:TYR:C	2.74	0.45
1:C:44:LEU:HD21	1:C:62:LEU:HD12	1.97	0.45
1:D:39:VAL:O	1:E:108:ILE:HG22	2.17	0.45
1:F:238:VAL:HG11	1:F:248:ARG:NH2	2.24	0.45
1:G:155:PHE:HA	1:G:161:GLY:N	2.32	0.45
1:G:158:GLY:HA2	1:G:161:GLY:O	2.17	0.45
1:G:308:PHE:HD1	1:G:410:ARG:HD2	1.82	0.45
1:I:386:GLU:HG3	1:I:387:ARG:HG3	1.99	0.45
1:J:41:LEU:HD13	1:J:66:VAL:HG12	1.99	0.45
1:J:87:LEU:O	1:J:87:LEU:HD13	2.17	0.45
1:J:181:PHE:CE1	1:J:590:PRO:HD2	2.52	0.45
1:L:470:PHE:HA	1:L:517:ILE:HD11	1.99	0.45
1:A:109:PRO:HG3	1:F:66:VAL:HG13	1.97	0.45
1:A:170:SER:HA	3:A:1001:ADP:O2B	2.17	0.45
1:C:473:LYS:HE3	1:C:515:LEU:O	2.16	0.45
1:D:274:GLY:O	1:D:423:ARG:NH2	2.44	0.45
1:E:153:PHE:CE2	1:E:157:ASN:HB3	2.52	0.45
1:G:20:GLY:HA3	1:I:70:HIS:HB2	1.99	0.45
1:L:396:VAL:HB	1:L:404:LEU:HD11	1.99	0.45
1:A:188:ARG:NH2	1:A:260:ARG:HB2	2.31	0.45
1:D:225:ASP:HB3	1:D:284:ARG:HH12	1.82	0.45
1:E:58:ARG:H	1:E:104:PRO:HD3	1.81	0.45
1:F:248:ARG:HH11	1:F:589:TYR:C	2.25	0.45
1:K:164:ILE:HD13	1:K:182:LEU:HD13	1.98	0.45
1:K:525:THR:HG22	1:K:527:SER:H	1.82	0.45
1:L:417:TYR:CD2	1:L:454:SER:HB2	2.51	0.45
1:H:415:GLN:O	1:H:419:SER:HB2	2.17	0.45
1:B:281:THR:HB	1:B:284:ARG:O	2.16	0.45
1:D:44:LEU:HD21	1:D:62:LEU:HD12	1.98	0.45
1:D:350:GLU:CG	1:D:351:ASP:N	2.77	0.45
1:E:81:ASP:HB3	1:E:86:LEU:HD12	1.98	0.45
1:F:269:ARG:CA	1:F:280:GLN:HG2	2.46	0.45
1:I:291:PHE:CD2	1:I:291:PHE:O	2.70	0.45
1:J:566:ALA:HA	1:J:569:LEU:CD1	2.47	0.45
1:L:51:LYS:HG2	1:L:52:PRO:HD2	1.98	0.45
1:H:331:LEU:HD23	1:H:342:LEU:HD21	1.99	0.45
1:A:416:LYS:HG3	1:A:417:TYR:CE1	2.52	0.45
1:B:228:ASN:ND2	1:B:600:GLU:OE1	2.49	0.45
1:D:149:LEU:HD22	1:D:587:VAL:HG11	1.99	0.45
1:D:269:ARG:HB2	1:D:278:VAL:O	2.17	0.45
1:G:29:PHE:CZ	1:G:47:VAL:HG11	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:238:VAL:HG11	1:I:248:ARG:CZ	2.47	0.45
1:J:69:ARG:HB2	1:J:92:SER:OG	2.17	0.45
1:J:307:VAL:HG11	1:J:411:LEU:HD23	1.99	0.45
1:K:175:LYS:NZ	1:K:523:GLN:C	2.75	0.45
1:L:153:PHE:CD2	1:L:195:THR:HG21	2.51	0.45
1:L:396:VAL:CG1	1:L:404:LEU:HD11	2.47	0.45
1:H:352:SER:HB2	1:H:385:GLU:OE2	2.17	0.44
1:A:87:LEU:C	1:A:87:LEU:CD2	2.89	0.44
1:A:221:LEU:HD23	1:A:221:LEU:HA	1.78	0.44
1:A:248:ARG:HB2	1:A:590:PRO:HG3	1.98	0.44
1:A:548:ALA:HB2	1:B:556:ARG:HB2	1.99	0.44
1:E:101:ARG:NH1	1:E:132:LYS:HE2	2.26	0.44
1:E:143:LEU:HD12	1:E:143:LEU:O	2.15	0.44
1:F:170:SER:OG	1:F:524:GLN:OE1	2.17	0.44
1:G:335:GLN:CD	1:G:343:ILE:H	2.24	0.44
1:I:515:LEU:HD12	1:I:515:LEU:O	2.16	0.44
1:J:82:VAL:HG22	1:J:87:LEU:CD2	2.47	0.44
1:J:397:LEU:HD23	1:L:401:PRO:HB2	1.99	0.44
1:K:248:ARG:CA	1:K:251:LEU:HD13	2.44	0.44
1:L:47:VAL:HG13	1:L:59:PHE:HB2	1.99	0.44
1:H:155:PHE:CD1	1:H:579:PRO:HG2	2.53	0.44
1:H:489:LEU:HA	1:H:489:LEU:HD23	1.80	0.44
1:A:388:GLU:O	1:A:388:GLU:CG	2.65	0.44
1:C:588:ASN:HD22	1:C:588:ASN:N	2.16	0.44
1:D:161:GLY:CA	1:D:513:ARG:CZ	2.95	0.44
1:I:82:VAL:HA	1:I:87:LEU:HB3	1.98	0.44
1:K:362:SER:HB3	1:K:366:GLY:CA	2.47	0.44
1:L:71:GLU:CG	1:L:92:SER:HB3	2.48	0.44
1:E:269:ARG:HB2	1:E:278:VAL:O	2.17	0.44
1:F:221:LEU:HA	1:F:221:LEU:HD23	1.66	0.44
1:G:107:PHE:CB	1:I:41:LEU:HB2	2.47	0.44
1:I:263:GLN:NE2	1:I:265:LEU:HD21	2.32	0.44
1:I:344:VAL:HG11	1:I:378:TYR:CE2	2.52	0.44
1:I:511:ARG:NH1	1:K:456:HIS:CE1	2.76	0.44
1:J:218:GLY:CA	1:J:451:HIS:CG	3.00	0.44
1:L:164:ILE:HD13	1:L:182:LEU:HD13	2.00	0.44
1:L:189:SER:O	1:L:194:ARG:NH2	2.48	0.44
1:L:566:ALA:HA	1:L:569:LEU:CG	2.45	0.44
1:A:86:LEU:C	1:A:86:LEU:HD13	2.43	0.44
1:C:192:MET:HB2	1:C:206:THR:HB	1.98	0.44
1:D:228:ASN:HD22	1:D:231:MET:N	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:269:ARG:HB2	1:F:278:VAL:HG23	2.00	0.44
1:G:236:ASP:O	1:G:240:ARG:HG2	2.17	0.44
1:I:269:ARG:HD3	1:I:280:GLN:HA	1.99	0.44
1:L:417:TYR:CE2	1:L:454:SER:HB2	2.53	0.44
1:L:597:ARG:HG2	1:L:598:ARG:H	1.80	0.44
1:H:168:GLY:O	1:H:524:GLN:HA	2.17	0.44
1:H:489:LEU:HD13	1:H:533:ILE:HG21	2.00	0.44
1:A:87:LEU:HD23	1:A:88:PRO:N	2.32	0.44
1:B:436:PRO:O	1:B:436:PRO:HG2	2.17	0.44
1:B:478:ARG:HB2	1:B:515:LEU:O	2.16	0.44
1:D:248:ARG:HD2	1:D:590:PRO:HA	1.98	0.44
1:E:58:ARG:HB2	1:E:103:ASP:CB	2.47	0.44
1:E:214:PHE:CD2	1:E:462:VAL:HG22	2.52	0.44
1:E:525:THR:HG22	1:E:527:SER:H	1.82	0.44
1:F:371:THR:OG1	1:F:373:GLU:OE1	2.35	0.44
1:F:469:VAL:O	1:F:473:LYS:HG2	2.17	0.44
1:G:265:LEU:HA	1:G:289:THR:O	2.17	0.44
1:I:33:VAL:CG1	1:I:93:TYR:CD2	3.00	0.44
1:I:41:LEU:C	1:I:63:VAL:HG12	2.30	0.44
1:I:59:PHE:HZ	1:I:108:ILE:O	2.01	0.44
1:I:173:ALA:HB2	1:I:544:ARG:H	1.82	0.44
1:I:215:ASN:CB	1:I:221:LEU:HB2	2.47	0.44
1:I:372:PHE:CE2	1:I:376:ILE:HD11	2.52	0.44
1:J:213:ILE:CD1	1:J:221:LEU:CD1	2.95	0.44
1:L:155:PHE:HA	1:L:161:GLY:HA3	2.00	0.44
1:L:423:ARG:HD3	1:L:426:LEU:HD11	2.00	0.44
1:A:143:LEU:HB3	1:A:587:VAL:HG12	1.99	0.44
1:B:473:LYS:CB	1:B:515:LEU:HG	2.48	0.44
1:C:199:SER:CB	1:C:203:GLN:HB2	2.48	0.44
1:C:269:ARG:HB2	1:C:278:VAL:HG23	1.99	0.44
1:C:326:GLU:CG	1:C:330:ARG:NH1	2.81	0.44
1:C:587:VAL:C	1:C:588:ASN:HD22	2.26	0.44
1:E:294:THR:HA	1:E:423:ARG:O	2.17	0.44
1:E:412:ARG:O	1:E:415:GLN:HG2	2.17	0.44
1:G:460:PHE:O	1:G:464:VAL:HG13	2.18	0.44
1:I:156:ILE:O	1:I:156:ILE:HG22	2.17	0.44
1:I:228:ASN:HD21	1:I:600:GLU:HB3	1.81	0.44
1:I:320:VAL:HG22	1:I:399:GLN:HG3	1.99	0.44
1:K:158:GLY:HA2	1:K:161:GLY:O	2.17	0.44
1:K:174:THR:OG1	1:K:174:THR:O	2.35	0.44
1:K:472:TYR:CE1	1:K:476:VAL:HG21	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:230:ARG:H	1:L:230:ARG:HG2	1.58	0.44
1:H:17:MET:HE1	1:G:83:VAL:HG21	1.99	0.44
1:H:153:PHE:CE2	1:H:157:ASN:HB3	2.52	0.44
1:A:396:VAL:CG2	1:A:404:LEU:HD11	2.48	0.44
1:B:344:VAL:HG11	1:B:378:TYR:CE2	2.52	0.44
1:B:412:ARG:HA	1:B:412:ARG:HD3	1.85	0.44
1:C:248:ARG:NH1	1:C:589:TYR:C	2.75	0.44
1:D:149:LEU:HD12	1:D:150:PRO:HD2	1.98	0.44
1:E:156:ILE:O	1:E:156:ILE:HG22	2.18	0.44
1:G:556:ARG:HB2	1:I:548:ALA:CB	2.48	0.44
1:J:21:THR:CG2	1:L:79:VAL:HG21	2.43	0.44
1:J:291:PHE:HA	1:J:434:TYR:O	2.16	0.44
1:K:227:PRO:HA	1:K:258:PRO:HG3	2.00	0.44
1:K:298:PHE:C	1:K:298:PHE:HD1	2.25	0.44
1:K:495:ARG:HH21	1:K:527:SER:C	2.26	0.44
1:H:108:ILE:HG22	1:G:40:GLY:HA2	1.99	0.44
1:A:42:ASP:OD2	1:A:586:LEU:HD22	2.18	0.44
1:A:331:LEU:HD21	1:A:344:VAL:HG12	2.00	0.44
1:A:353:GLU:HA	1:A:353:GLU:OE2	2.18	0.44
1:B:474:GLU:HG3	1:B:515:LEU:HD21	1.99	0.44
1:D:423:ARG:NH1	1:D:426:LEU:HD21	2.33	0.44
1:G:530:GLU:HB3	1:G:533:ILE:HD13	1.99	0.44
1:J:79:VAL:HG21	1:K:19:LEU:HD12	2.00	0.44
1:K:362:SER:HB3	1:K:366:GLY:N	2.32	0.44
1:K:542:VAL:HG12	1:K:543:GLY:O	2.17	0.44
1:L:41:LEU:HD13	1:L:66:VAL:HG12	2.00	0.44
1:B:369:LEU:HD13	1:B:375:LEU:HD12	2.00	0.44
1:C:149:LEU:HD22	1:C:587:VAL:HG11	2.00	0.44
1:E:67:ARG:HA	1:F:24:VAL:O	2.17	0.44
1:E:125:ALA:HB1	1:E:130:ALA:HB3	2.00	0.44
1:F:203:GLN:O	1:F:203:GLN:HG3	2.18	0.44
1:G:478:ARG:HG3	1:G:515:LEU:C	2.43	0.44
1:I:472:TYR:CZ	1:I:476:VAL:HG21	2.53	0.44
1:J:60:TYR:CE2	1:J:103:ASP:HB2	2.49	0.44
1:J:282:ASP:HB3	1:K:202:ARG:HH22	1.82	0.44
1:K:349:PHE:CD2	1:K:349:PHE:O	2.70	0.44
1:H:231:MET:HE2	1:H:231:MET:HB3	1.88	0.43
1:B:286:GLU:O	1:B:288:VAL:HG23	2.18	0.43
1:B:443:ILE:HD13	1:B:443:ILE:HA	1.84	0.43
1:C:188:ARG:HH22	1:C:259:PHE:HA	1.83	0.43
1:C:242:LYS:CB	1:C:244:LEU:CD1	2.96	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:176:THR:HB	3:E:1001:ADP:O1A	2.18	0.43
1:E:495:ARG:NE	1:E:527:SER:O	2.51	0.43
1:I:215:ASN:HA	1:I:221:LEU:HD12	2.00	0.43
1:K:191:VAL:HG22	1:K:191:VAL:O	2.18	0.43
1:K:283:GLN:H	1:K:283:GLN:HG2	1.57	0.43
1:K:315:LEU:CB	1:K:317:LEU:HD13	2.41	0.43
1:L:82:VAL:HG11	1:L:89:ALA:HB3	1.99	0.43
1:H:268:PRO:HG3	1:H:292:VAL:HG12	1.99	0.43
1:A:153:PHE:HE2	1:A:195:THR:HG21	1.80	0.43
1:A:347:TRP:CD1	1:A:381:TYR:CD2	3.06	0.43
1:B:178:TYR:CE2	1:B:541:VAL:HG11	2.52	0.43
1:C:326:GLU:HG3	1:C:330:ARG:NH1	2.32	0.43
1:D:57:VAL:HG13	1:D:104:PRO:HD2	1.99	0.43
1:E:167:SER:O	1:E:542:VAL:HA	2.17	0.43
1:F:135:GLU:HB2	1:F:194:ARG:HB3	2.00	0.43
1:G:331:LEU:HD21	1:G:344:VAL:HG12	2.01	0.43
1:I:49:THR:OG1	1:I:114:ASP:OD2	2.31	0.43
1:J:282:ASP:HB3	1:K:202:ARG:NH2	2.33	0.43
1:K:432:GLU:O	1:K:435:ARG:HG2	2.18	0.43
1:L:248:ARG:HH11	1:L:590:PRO:HA	1.83	0.43
1:L:291:PHE:HA	1:L:434:TYR:O	2.18	0.43
1:L:473:LYS:CB	1:L:515:LEU:HG	2.49	0.43
1:L:603:ASP:O	1:L:604:LEU:HD13	2.18	0.43
1:H:128:LEU:HD11	1:H:143:LEU:HD11	1.99	0.43
1:H:191:VAL:O	1:H:195:THR:HG22	2.19	0.43
1:H:319:PHE:CZ	1:G:315:LEU:CD2	3.01	0.43
1:H:405:ARG:NH2	1:L:326:GLU:HG2	2.33	0.43
1:H:505:LEU:HD23	1:H:505:LEU:HA	1.85	0.43
1:B:133:MET:SD	1:B:150:PRO:HB2	2.57	0.43
1:D:248:ARG:HH11	1:D:589:TYR:C	2.26	0.43
1:E:133:MET:HG2	1:E:152:ASN:HB2	2.00	0.43
1:E:489:LEU:HA	1:E:489:LEU:HD23	1.85	0.43
1:G:202:ARG:HB3	1:G:202:ARG:HH11	1.80	0.43
1:I:142:LEU:HD23	1:I:142:LEU:HA	1.88	0.43
1:I:149:LEU:HD21	1:I:576:VAL:HG21	1.99	0.43
1:J:269:ARG:HA	1:J:280:GLN:HG2	1.99	0.43
1:K:60:TYR:HE2	1:K:103:ASP:HB2	1.83	0.43
1:K:215:ASN:HD21	1:K:451:HIS:CD2	2.33	0.43
1:K:387:ARG:HB2	1:K:390:GLU:HG2	1.99	0.43
1:K:566:ALA:HA	1:K:569:LEU:HD13	1.99	0.43
1:H:57:VAL:HG13	1:H:104:PRO:HD2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:307:VAL:HG11	1:H:411:LEU:HD23	1.99	0.43
1:A:269:ARG:CA	1:A:280:GLN:HG2	2.47	0.43
1:B:165:ASN:ND2	1:B:523:GLN:HE22	2.15	0.43
1:B:368:ASN:ND2	1:B:370:GLN:HG2	2.31	0.43
1:B:597:ARG:HB3	1:B:600:GLU:HG3	2.00	0.43
1:D:221:LEU:HD23	1:D:221:LEU:HA	1.83	0.43
1:D:440:ARG:HB3	1:D:443:ILE:CG1	2.49	0.43
1:F:175:LYS:HZ3	1:F:524:GLN:HA	1.82	0.43
1:G:183:LEU:HD23	1:G:183:LEU:HA	1.90	0.43
1:I:227:PRO:HA	1:I:258:PRO:HG3	2.01	0.43
1:J:331:LEU:HD12	1:J:331:LEU:HA	1.86	0.43
1:K:80:GLU:HG3	1:K:81:ASP:H	1.84	0.43
1:K:263:GLN:NE2	1:K:265:LEU:HD21	2.33	0.43
1:H:83:VAL:HG21	1:L:17:MET:HE1	2.00	0.43
1:A:226:LYS:HB3	1:A:226:LYS:HE3	1.77	0.43
1:G:392:ASP:O	1:G:395:TRP:N	2.50	0.43
1:I:59:PHE:HD2	1:I:99:VAL:HG11	1.84	0.43
1:K:163:HIS:CB	1:K:519:LEU:O	2.65	0.43
1:K:473:LYS:HZ2	1:K:473:LYS:HA	1.83	0.43
1:L:348:GLN:H	1:L:348:GLN:CD	2.26	0.43
1:A:227:PRO:HA	1:A:258:PRO:HG3	2.01	0.43
1:E:163:HIS:HB3	1:E:519:LEU:O	2.18	0.43
1:G:24:VAL:CG1	1:G:110:PRO:HD2	2.49	0.43
1:G:142:LEU:HD23	1:G:142:LEU:HA	1.85	0.43
1:G:525:THR:HG22	1:G:527:SER:H	1.83	0.43
1:I:29:PHE:CZ	1:I:47:VAL:CG1	3.01	0.43
1:J:131:ASP:O	1:J:134:GLU:HG2	2.19	0.43
1:A:19:LEU:HD12	1:A:19:LEU:HA	1.85	0.43
1:C:24:VAL:O	1:C:109:PRO:HB3	2.19	0.43
1:D:62:LEU:HD23	1:D:63:VAL:O	2.19	0.43
1:G:184:HIS:NE2	1:G:255:PRO:O	2.45	0.43
1:G:338:LYS:HE3	1:G:428:PRO:HG2	2.00	0.43
1:I:88:PRO:O	1:I:88:PRO:HG2	2.19	0.43
1:I:320:VAL:CG2	1:I:399:GLN:HG3	2.47	0.43
1:I:426:LEU:HB3	1:I:430:GLN:HE21	1.83	0.43
1:L:106:ASN:HB3	1:L:108:ILE:HG12	1.99	0.43
1:L:269:ARG:CA	1:L:280:GLN:HG2	2.48	0.43
1:L:469:VAL:O	1:L:473:LYS:HG2	2.19	0.43
1:H:76:GLU:HG2	1:L:71:GLU:OE2	2.19	0.43
1:H:218:GLY:HA2	1:H:451:HIS:CG	2.53	0.43
1:A:193:ASP:OD2	1:A:206:THR:HG21	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:24:VAL:O	1:B:109:PRO:HB3	2.19	0.43
1:B:70:HIS:HB2	1:C:20:GLY:HA3	2.01	0.43
1:B:248:ARG:HD2	1:B:590:PRO:HA	2.00	0.43
1:B:349:PHE:CB	1:B:352:SER:HB3	2.43	0.43
1:F:155:PHE:HA	1:F:161:GLY:CA	2.49	0.43
1:F:156:ILE:C	1:F:162:GLY:O	2.62	0.43
1:F:231:MET:HE1	1:F:256:ALA:HB1	1.99	0.43
1:F:525:THR:HG22	1:F:527:SER:H	1.83	0.43
1:G:155:PHE:CD1	1:G:579:PRO:HG2	2.53	0.43
1:G:515:LEU:HD12	1:G:515:LEU:HA	1.81	0.43
1:J:396:VAL:HG23	1:J:404:LEU:HD21	2.01	0.43
1:K:304:LEU:N	1:K:305:PRO:CD	2.81	0.43
1:K:419:SER:N	1:K:420:PRO:CD	2.81	0.43
1:L:317:LEU:O	1:L:321:ILE:HG13	2.18	0.43
1:B:467:ARG:HD3	1:B:467:ARG:HA	1.74	0.43
1:C:70:HIS:HB3	1:C:73:VAL:HG21	2.00	0.43
1:C:163:HIS:CD2	1:C:163:HIS:N	2.87	0.43
1:C:495:ARG:NE	1:C:527:SER:O	2.52	0.43
1:D:105:GLU:O	1:D:105:GLU:HG3	2.19	0.43
1:E:172:VAL:HG11	1:E:544:ARG:HD2	2.01	0.43
1:E:478:ARG:HG3	1:E:516:GLY:N	2.34	0.43
1:I:21:THR:HG21	1:K:76:GLU:HA	2.00	0.43
1:J:107:PHE:HB3	1:L:41:LEU:HB2	2.01	0.43
1:J:394:LYS:O	1:J:397:LEU:HD11	2.19	0.43
1:L:416:LYS:H	1:L:416:LYS:HG2	1.61	0.43
1:A:131:ASP:O	1:A:134:GLU:HG2	2.19	0.43
1:C:263:GLN:NE2	1:C:265:LEU:HD21	2.34	0.43
1:F:515:LEU:HD12	1:F:515:LEU:HA	1.76	0.43
1:G:105:GLU:OE2	1:I:570:GLN:HB2	2.19	0.43
1:I:107:PHE:CB	1:K:41:LEU:HB2	2.48	0.43
1:K:29:PHE:CZ	1:K:47:VAL:HG11	2.54	0.43
1:K:173:ALA:HB2	1:K:544:ARG:N	2.34	0.43
1:L:396:VAL:HG12	1:L:404:LEU:CD1	2.49	0.43
1:A:394:LYS:HB2	1:A:394:LYS:HE3	1.80	0.42
1:C:199:SER:HB3	1:C:203:GLN:HB2	2.01	0.42
1:C:291:PHE:HA	1:C:434:TYR:O	2.18	0.42
1:D:350:GLU:CG	1:D:351:ASP:H	2.29	0.42
1:E:416:LYS:HG3	1:E:417:TYR:CE1	2.54	0.42
1:E:478:ARG:HD2	1:E:514:SER:O	2.19	0.42
1:F:42:ASP:OD2	1:F:586:LEU:HD22	2.18	0.42
1:G:412:ARG:O	1:G:415:GLN:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:247:ASP:OD1	1:I:247:ASP:N	2.51	0.42
1:L:165:ASN:HD21	1:L:523:GLN:NE2	2.17	0.42
1:A:151:LEU:HD23	1:A:151:LEU:HA	1.68	0.42
1:B:488:GLU:OE2	1:B:491:LYS:HD3	2.19	0.42
1:D:161:GLY:HA3	1:D:513:ARG:CZ	2.49	0.42
1:E:351:ASP:C	1:E:353:GLU:H	2.26	0.42
1:F:196:ALA:HB1	1:F:204:SER:HA	2.00	0.42
1:F:242:LYS:CB	1:F:244:LEU:CD1	2.97	0.42
1:G:131:ASP:OD1	1:G:131:ASP:N	2.46	0.42
1:G:556:ARG:HB2	1:I:548:ALA:HB2	2.01	0.42
1:I:267:PRO:HB3	1:I:421:LEU:HD21	2.01	0.42
1:I:349:PHE:HB3	1:I:352:SER:HB3	2.01	0.42
1:I:588:ASN:ND2	1:I:588:ASN:C	2.73	0.42
1:L:308:PHE:CZ	1:L:411:LEU:HD11	2.53	0.42
1:L:415:GLN:O	1:L:419:SER:HB2	2.18	0.42
1:H:236:ASP:O	1:H:240:ARG:HG2	2.18	0.42
1:H:478:ARG:HG3	1:H:515:LEU:C	2.43	0.42
1:A:478:ARG:HG3	1:A:515:LEU:C	2.45	0.42
1:C:418:LEU:HD21	1:C:457:ALA:HA	2.01	0.42
1:D:188:ARG:NH2	1:D:260:ARG:HG3	2.34	0.42
1:D:418:LEU:HD23	1:D:421:LEU:HD12	2.00	0.42
1:F:310:ASP:OD2	1:F:314:SER:HB3	2.19	0.42
1:F:320:VAL:HG21	1:F:403:THR:HG22	2.02	0.42
1:G:64:ASP:OD1	1:G:96:ARG:HD2	2.19	0.42
1:I:349:PHE:CB	1:I:352:SER:HB3	2.49	0.42
1:J:268:PRO:HG3	1:J:292:VAL:HG12	2.01	0.42
1:K:225:ASP:O	1:K:258:PRO:CB	2.67	0.42
1:K:251:LEU:HD12	1:K:251:LEU:N	2.35	0.42
1:K:277:ILE:HG21	1:K:434:TYR:CE2	2.54	0.42
1:A:174:THR:HA	3:A:1001:ADP:O5'	2.19	0.42
1:D:307:VAL:HG11	1:D:411:LEU:HD23	2.01	0.42
1:E:163:HIS:HE1	1:E:508:ILE:O	2.03	0.42
1:E:174:THR:HA	3:E:1001:ADP:H5'2	2.01	0.42
1:E:375:LEU:O	1:E:379:LEU:HG	2.19	0.42
1:E:405:ARG:HA	1:E:408:THR:HB	2.01	0.42
1:F:60:TYR:HE2	1:F:103:ASP:HB2	1.84	0.42
1:F:155:PHE:HA	1:F:161:GLY:HA3	2.01	0.42
1:F:294:THR:HA	1:F:423:ARG:O	2.19	0.42
1:I:33:VAL:HG11	1:I:93:TYR:CD2	2.53	0.42
1:K:57:VAL:HG22	1:K:104:PRO:HG2	2.01	0.42
1:K:386:GLU:CG	1:K:387:ARG:HG3	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:248:ARG:O	1:H:252:LEU:HD13	2.19	0.42
1:A:17:MET:CE	1:F:83:VAL:HG11	2.47	0.42
1:C:81:ASP:HB3	1:C:86:LEU:HB2	2.02	0.42
1:C:269:ARG:HB2	1:C:278:VAL:O	2.19	0.42
1:C:294:THR:HA	1:C:423:ARG:O	2.20	0.42
1:C:560:GLN:HA	1:C:563:ARG:HG3	2.01	0.42
1:D:133:MET:SD	1:D:150:PRO:HB2	2.60	0.42
1:E:335:GLN:NE2	1:E:343:ILE:O	2.52	0.42
1:E:387:ARG:C	1:E:388:GLU:OE1	2.63	0.42
1:E:478:ARG:HG3	1:E:515:LEU:C	2.43	0.42
1:F:354:THR:HA	1:F:355:PRO:HD2	1.84	0.42
1:I:466:LEU:HB3	1:I:504:VAL:HG21	2.01	0.42
1:H:188:ARG:HH22	1:H:260:ARG:HG2	1.83	0.42
1:A:310:ASP:OD2	1:A:314:SER:HB3	2.19	0.42
1:A:349:PHE:CE1	1:A:356:PRO:CB	3.03	0.42
1:C:221:LEU:HA	1:C:221:LEU:HD23	1.74	0.42
1:E:44:LEU:HD21	1:E:62:LEU:HD12	2.02	0.42
1:F:265:LEU:HA	1:F:289:THR:O	2.19	0.42
1:F:310:ASP:OD2	1:F:312:SER:HB2	2.20	0.42
1:I:530:GLU:HG3	1:I:532:ARG:H	1.85	0.42
1:K:386:GLU:HB3	1:K:391:GLY:HA2	2.02	0.42
1:K:387:ARG:O	1:K:388:GLU:CG	2.65	0.42
1:K:387:ARG:O	1:K:390:GLU:HG2	2.19	0.42
1:K:396:VAL:O	1:K:396:VAL:CG2	2.60	0.42
1:B:215:ASN:HB3	1:B:449:ASP:HA	2.02	0.42
1:B:277:ILE:O	1:B:277:ILE:HG13	2.20	0.42
1:B:293:PHE:CZ	1:B:464:VAL:CG2	3.03	0.42
1:E:215:ASN:HB3	1:E:449:ASP:HA	2.02	0.42
1:E:224:LEU:HD12	1:E:445:LEU:HD21	2.00	0.42
1:F:190:GLY:O	1:F:193:ASP:HB2	2.20	0.42
1:I:376:ILE:CD1	1:I:411:LEU:HB3	2.45	0.42
1:J:284:ARG:O	1:J:288:VAL:HG21	2.20	0.42
1:J:326:GLU:CG	1:J:330:ARG:NH1	2.82	0.42
1:K:288:VAL:HG13	1:K:288:VAL:O	2.19	0.42
1:A:264:LEU:HD23	1:A:447:VAL:HB	2.01	0.42
1:G:188:ARG:NH2	1:G:260:ARG:HG3	2.35	0.42
1:I:397:LEU:HB3	1:K:401:PRO:CB	2.50	0.42
1:J:335:GLN:CD	1:J:343:ILE:H	2.28	0.42
1:L:218:GLY:HA2	1:L:451:HIS:CG	2.53	0.42
1:L:372:PHE:HD2	1:L:415:GLN:HB2	1.85	0.42
1:A:265:LEU:HA	1:A:289:THR:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:597:ARG:HG2	1:C:600:GLU:CG	2.50	0.42
1:E:103:ASP:HB3	1:E:104:PRO:HD3	2.02	0.42
1:E:269:ARG:HB2	1:E:278:VAL:HG23	2.02	0.42
1:G:31:PHE:CE2	1:G:116:VAL:HG11	2.55	0.42
1:K:228:ASN:HB2	1:K:595:ALA:HA	2.01	0.42
1:K:354:THR:OG1	1:K:355:PRO:HD2	2.19	0.42
1:K:495:ARG:HH21	1:K:527:SER:CA	2.29	0.42
1:L:515:LEU:HD12	1:L:515:LEU:HA	1.75	0.42
1:A:165:ASN:OD1	1:A:523:GLN:NE2	2.38	0.42
1:B:263:GLN:NE2	1:B:265:LEU:HD21	2.35	0.42
1:D:249:TYR:OH	1:D:591:PHE:O	2.28	0.42
1:F:155:PHE:CD1	1:F:161:GLY:HA3	2.54	0.42
1:F:412:ARG:O	1:F:415:GLN:HG2	2.20	0.42
1:G:107:PHE:HB3	1:I:41:LEU:HB2	2.01	0.42
1:G:221:LEU:HD22	1:G:224:LEU:HD11	2.00	0.42
1:J:70:HIS:HB2	1:K:20:GLY:HA3	2.02	0.42
1:J:236:ASP:O	1:J:240:ARG:HG2	2.20	0.42
1:K:369:LEU:CD2	1:K:374:GLN:HB3	2.50	0.42
1:K:513:ARG:CB	1:K:513:ARG:CZ	2.98	0.42
1:L:223:PHE:HA	1:L:284:ARG:NH1	2.35	0.42
1:L:375:LEU:O	1:L:379:LEU:HG	2.19	0.42
1:A:473:LYS:HG3	1:A:517:ILE:CG1	2.50	0.41
1:C:249:TYR:OH	1:C:591:PHE:O	2.29	0.41
1:D:41:LEU:HB2	1:E:107:PHE:HB3	2.02	0.41
1:D:326:GLU:CG	1:D:330:ARG:NH1	2.82	0.41
1:E:169:ILE:N	1:E:544:ARG:O	2.48	0.41
1:F:597:ARG:HB3	1:F:600:GLU:HG3	2.01	0.41
1:G:248:ARG:HB2	1:G:590:PRO:HG3	2.02	0.41
1:I:210:ARG:HG2	1:I:210:ARG:HH11	1.85	0.41
1:K:173:ALA:HB2	1:K:544:ARG:H	1.84	0.41
1:K:472:TYR:CE1	1:K:476:VAL:HB	2.54	0.41
1:A:242:LYS:NZ	1:A:588:ASN:OD1	2.54	0.41
1:B:486:LEU:O	1:B:521:GLY:HA2	2.20	0.41
1:C:166:ILE:O	1:C:522:ALA:HA	2.20	0.41
1:C:327:LYS:HD3	1:C:327:LYS:HA	1.86	0.41
1:E:315:LEU:HG	1:E:316:ASN:H	1.84	0.41
1:E:525:THR:HG21	1:E:549:GLU:OE1	2.20	0.41
1:F:356:PRO:N	1:F:356:PRO:C	2.67	0.41
1:G:393:PRO:O	1:G:397:LEU:HD12	2.20	0.41
1:I:570:GLN:HG3	1:I:571:PRO:HD2	2.01	0.41
1:K:473:LYS:HA	1:K:476:VAL:HG12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:82:VAL:CG1	1:L:89:ALA:HB3	2.50	0.41
1:L:192:MET:O	1:L:196:ALA:CB	2.65	0.41
1:L:343:ILE:HD13	1:L:362:SER:CB	2.50	0.41
1:L:394:LYS:HE3	1:L:394:LYS:HB3	1.82	0.41
1:H:221:LEU:HD23	1:H:221:LEU:HA	1.65	0.41
1:D:486:LEU:HD12	1:D:486:LEU:HA	1.86	0.41
1:E:530:GLU:HB3	1:E:533:ILE:HD13	2.02	0.41
1:J:16:GLY:HA2	1:J:34:SER:OG	2.20	0.41
1:J:216:VAL:HG21	1:J:492:TYR:OH	2.20	0.41
1:J:267:PRO:HB3	1:J:421:LEU:HD21	2.03	0.41
1:J:418:LEU:HD23	1:J:421:LEU:HD12	2.02	0.41
1:K:223:PHE:HA	1:K:284:ARG:NH1	2.35	0.41
1:K:456:HIS:ND1	1:K:456:HIS:N	2.68	0.41
1:H:515:LEU:HA	1:H:515:LEU:HD12	1.83	0.41
1:A:219:GLU:HG2	1:A:222:LEU:HD22	2.02	0.41
1:A:335:GLN:CD	1:A:343:ILE:H	2.29	0.41
1:B:81:ASP:HB3	1:B:86:LEU:HB2	2.02	0.41
1:C:51:LYS:HG2	1:C:52:PRO:HD2	2.02	0.41
1:C:131:ASP:OD1	1:C:131:ASP:N	2.49	0.41
1:C:264:LEU:HD23	1:C:447:VAL:HB	2.02	0.41
1:E:213:ILE:CG1	1:E:485:VAL:HB	2.40	0.41
1:E:304:LEU:HD22	1:E:324:ILE:HG22	2.01	0.41
1:E:545:LEU:HD11	1:E:555:TYR:CD1	2.55	0.41
1:F:47:VAL:HG23	1:F:115:HIS:O	2.21	0.41
1:G:291:PHE:HD2	1:G:436:PRO:HG3	1.85	0.41
1:I:40:GLY:N	1:I:43:ASP:OD2	2.50	0.41
1:K:136:ALA:CA	1:K:195:THR:HG22	2.49	0.41
1:K:213:ILE:HD13	1:K:221:LEU:HD21	1.97	0.41
1:L:252:LEU:HD22	1:L:254:LEU:HD12	2.02	0.41
1:L:412:ARG:O	1:L:415:GLN:HG2	2.20	0.41
1:B:248:ARG:O	1:B:252:LEU:HD12	2.20	0.41
1:B:299:CYS:HB2	1:B:332:ALA:HB2	2.01	0.41
1:B:320:VAL:HG22	1:B:399:GLN:HG2	2.02	0.41
1:C:292:VAL:HG21	1:C:426:LEU:CD1	2.50	0.41
1:F:149:LEU:HD22	1:F:587:VAL:HG11	2.01	0.41
1:F:268:PRO:HG3	1:F:292:VAL:HG12	2.03	0.41
1:F:387:ARG:O	1:F:390:GLU:HG2	2.21	0.41
1:G:470:PHE:CZ	1:G:507:ASP:HB3	2.55	0.41
1:I:597:ARG:HB3	1:I:600:GLU:HG3	2.03	0.41
1:K:156:ILE:O	1:K:518:ILE:HD12	2.19	0.41
1:K:227:PRO:HG3	1:K:258:PRO:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:223:PHE:O	1:L:595:ALA:HB3	2.21	0.41
1:L:331:LEU:HA	1:L:331:LEU:HD12	1.76	0.41
1:L:554:GLU:OE1	1:L:554:GLU:N	2.53	0.41
1:H:506:LEU:HD23	1:H:533:ILE:HD11	2.02	0.41
1:A:68:LYS:NZ	1:B:111:GLN:HG2	2.35	0.41
1:D:180:LEU:HD11	1:D:221:LEU:HD21	2.02	0.41
1:E:441:ARG:HD2	1:E:442:GLY:N	2.35	0.41
1:E:530:GLU:HG3	1:E:532:ARG:H	1.85	0.41
1:F:63:VAL:HA	1:F:96:ARG:O	2.20	0.41
1:F:217:LYS:HA	1:F:217:LYS:HD3	1.98	0.41
1:F:232:VAL:O	1:F:236:ASP:HB2	2.21	0.41
1:G:106:ASN:HD22	1:G:106:ASN:HA	1.58	0.41
1:I:104:PRO:O	1:I:104:PRO:HD2	2.21	0.41
1:J:392:ASP:OD1	1:J:393:PRO:HD2	2.20	0.41
1:K:263:GLN:HB2	1:K:443:ILE:HG21	2.02	0.41
1:K:267:PRO:CB	1:K:453:LEU:HD21	2.50	0.41
1:K:275:THR:HG23	1:K:425:ASP:OD2	2.21	0.41
1:L:41:LEU:HD12	1:L:41:LEU:HA	1.92	0.41
1:L:218:GLY:N	1:L:451:HIS:HB2	2.25	0.41
1:C:423:ARG:NH1	1:C:425:ASP:OD1	2.53	0.41
1:C:423:ARG:NH1	1:C:426:LEU:HD21	2.35	0.41
1:D:249:TYR:HB3	1:D:254:LEU:O	2.19	0.41
1:D:376:ILE:HD13	1:D:411:LEU:HB3	2.02	0.41
1:E:76:GLU:HB3	1:F:21:THR:HG21	2.03	0.41
1:E:182:LEU:HA	1:E:182:LEU:HD23	1.81	0.41
1:E:597:ARG:NH2	1:F:198:GLY:O	2.53	0.41
1:F:156:ILE:CA	1:F:162:GLY:O	2.68	0.41
1:G:111:GLN:HG3	1:I:91:VAL:HG11	2.02	0.41
1:G:223:PHE:CE1	1:G:284:ARG:HB2	2.56	0.41
1:I:210:ARG:HG2	1:I:210:ARG:NH1	2.36	0.41
1:J:354:THR:O	1:J:354:THR:OG1	2.38	0.41
1:J:403:THR:CA	1:K:319:PHE:HE1	2.33	0.41
1:K:483:PHE:CD1	1:K:518:ILE:HB	2.56	0.41
1:K:545:LEU:HA	1:K:545:LEU:HD23	1.80	0.41
1:L:71:GLU:HG2	1:L:92:SER:HB3	2.02	0.41
1:L:396:VAL:CB	1:L:404:LEU:HD11	2.51	0.41
1:L:570:GLN:O	1:L:573:THR:HB	2.20	0.41
1:A:469:VAL:O	1:A:473:LYS:HG2	2.19	0.41
1:B:292:VAL:HG21	1:B:426:LEU:HD11	2.02	0.41
1:E:405:ARG:O	1:E:409:ARG:N	2.39	0.41
1:G:21:THR:HG21	1:I:76:GLU:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:331:LEU:HD23	1:I:342:LEU:HD21	2.03	0.41
1:I:419:SER:N	1:I:420:PRO:CD	2.83	0.41
1:J:52:PRO:HB3	1:L:36:GLY:HA2	2.02	0.41
1:J:175:LYS:HZ3	1:J:524:GLN:HA	1.85	0.41
1:J:248:ARG:NH1	1:J:590:PRO:HA	2.35	0.41
1:J:294:THR:HA	1:J:423:ARG:O	2.21	0.41
1:K:26:PRO:HG3	1:K:108:ILE:C	2.46	0.41
1:K:73:VAL:O	1:K:73:VAL:CG2	2.67	0.41
1:K:215:ASN:HD22	1:K:451:HIS:HD2	1.63	0.41
1:K:495:ARG:NE	1:K:527:SER:O	2.51	0.41
1:H:213:ILE:HD12	1:H:485:VAL:HB	2.02	0.41
1:H:248:ARG:CB	1:H:590:PRO:HG3	2.51	0.41
1:A:548:ALA:CB	1:B:556:ARG:HB2	2.51	0.41
1:B:41:LEU:HD13	1:B:66:VAL:HG12	2.02	0.41
1:C:315:LEU:HD23	1:C:317:LEU:CD1	2.51	0.41
1:D:335:GLN:CD	1:D:343:ILE:H	2.28	0.41
1:D:412:ARG:O	1:D:415:GLN:HG2	2.21	0.41
1:E:416:LYS:HG3	1:E:417:TYR:CD1	2.55	0.41
1:F:142:LEU:HG	1:F:252:LEU:CD1	2.48	0.41
1:F:195:THR:HG23	1:F:203:GLN:NE2	2.35	0.41
1:F:269:ARG:HB2	1:F:278:VAL:O	2.20	0.41
1:G:51:LYS:HE3	1:G:55:THR:OG1	2.21	0.41
1:G:165:ASN:HD21	1:G:523:GLN:HE22	1.68	0.41
1:I:23:ASP:CG	1:K:69:ARG:HH21	2.28	0.41
1:I:202:ARG:HG2	1:I:478:ARG:NH2	2.35	0.41
1:I:268:PRO:CB	1:I:277:ILE:HG23	2.51	0.41
1:I:315:LEU:HD23	1:I:317:LEU:CD1	2.51	0.41
1:I:397:LEU:H	1:I:397:LEU:CD2	2.33	0.41
1:J:143:LEU:HD23	1:J:149:LEU:HB2	2.02	0.41
1:K:223:PHE:HE1	1:K:284:ARG:HB2	1.84	0.41
1:K:267:PRO:CG	1:K:453:LEU:HD21	2.49	0.41
1:K:362:SER:HB3	1:K:366:GLY:H	1.86	0.41
1:L:59:PHE:CD2	1:L:102:VAL:HG12	2.56	0.41
1:L:143:LEU:HD12	1:L:147:GLN:O	2.21	0.41
1:L:203:GLN:HG3	1:L:203:GLN:O	2.21	0.41
1:L:321:ILE:HG13	1:L:321:ILE:H	1.67	0.41
1:L:525:THR:HG21	1:L:549:GLU:OE1	2.21	0.41
1:H:242:LYS:HZ1	1:H:588:ASN:HD21	1.62	0.41
1:A:399:GLN:HB3	1:A:404:LEU:HD21	2.03	0.41
1:A:401:PRO:HA	1:A:404:LEU:HB2	2.02	0.41
1:B:221:LEU:HD23	1:B:221:LEU:HA	1.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:236:ASP:O	1:B:240:ARG:HG2	2.21	0.41
1:B:249:TYR:OH	1:B:591:PHE:O	2.30	0.41
1:C:294:THR:HB	1:C:340:THR:HB	2.03	0.41
1:D:201:GLY:HA2	1:D:204:SER:HG	1.86	0.41
1:E:174:THR:HG22	3:E:1001:ADP:C5'	2.50	0.41
1:F:495:ARG:NE	1:F:527:SER:O	2.54	0.41
1:G:24:VAL:HG12	1:G:110:PRO:HD2	2.03	0.41
1:I:304:LEU:N	1:I:305:PRO:CD	2.84	0.41
1:I:355:PRO:O	1:I:355:PRO:CD	2.69	0.41
1:J:403:THR:HA	1:K:319:PHE:HE1	1.86	0.41
1:K:111:GLN:N	1:K:114:ASP:OD2	2.53	0.41
1:K:223:PHE:CE1	1:K:284:ARG:HB2	2.56	0.41
1:K:259:PHE:HE1	1:K:594:TRP:CD2	2.39	0.41
1:L:203:GLN:O	1:L:203:GLN:CG	2.69	0.41
1:H:252:LEU:HD23	1:H:254:LEU:HD12	2.03	0.40
1:D:228:ASN:HD22	1:D:231:MET:H	1.68	0.40
1:E:70:HIS:HB3	1:E:73:VAL:HG22	2.03	0.40
1:F:331:LEU:HD12	1:F:331:LEU:HA	1.93	0.40
1:G:401:PRO:HA	1:G:404:LEU:HD12	2.02	0.40
1:I:51:LYS:HZ1	1:I:106:ASN:ND2	2.19	0.40
1:J:249:TYR:OH	1:J:591:PHE:O	2.35	0.40
1:J:349:PHE:CB	1:J:352:SER:CB	2.93	0.40
1:K:51:LYS:HB2	1:K:55:THR:O	2.22	0.40
1:K:135:GLU:CD	1:K:135:GLU:H	2.29	0.40
1:K:183:LEU:HD23	1:K:183:LEU:HA	1.85	0.40
1:K:364:LEU:HD12	1:K:364:LEU:HA	1.64	0.40
1:K:416:LYS:HG3	1:K:417:TYR:CE1	2.56	0.40
1:L:51:LYS:HB2	1:L:55:THR:O	2.21	0.40
1:L:68:LYS:HA	1:L:92:SER:O	2.20	0.40
1:L:155:PHE:CD1	1:L:579:PRO:HG2	2.57	0.40
1:L:301:ARG:NH2	1:L:468:GLU:OE2	2.54	0.40
1:A:36:GLY:HA2	1:B:52:PRO:HB3	2.02	0.40
1:A:163:HIS:CD2	1:A:163:HIS:H	2.39	0.40
1:C:418:LEU:HD23	1:C:421:LEU:HD12	2.02	0.40
1:J:19:LEU:HD12	1:J:19:LEU:HA	1.85	0.40
1:K:316:ASN:C	1:K:318:GLY:H	2.28	0.40
1:L:59:PHE:HZ	1:L:108:ILE:O	2.04	0.40
1:L:84:ALA:CB	1:L:86:LEU:HD21	2.51	0.40
1:L:267:PRO:HD3	1:L:449:ASP:O	2.20	0.40
1:L:320:VAL:CG1	1:L:399:GLN:HG2	2.50	0.40
1:L:386:GLU:HB3	1:L:391:GLY:HA2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:172:VAL:HG11	1:H:544:ARG:HD2	2.02	0.40
1:H:248:ARG:HH11	1:H:589:TYR:C	2.29	0.40
1:A:473:LYS:HG3	1:A:517:ILE:HD11	2.02	0.40
1:A:488:GLU:OE1	1:A:491:LYS:HD3	2.22	0.40
1:B:66:VAL:HG13	1:C:109:PRO:HG3	2.03	0.40
1:B:439:LEU:CD1	1:B:469:VAL:HG22	2.51	0.40
1:E:320:VAL:HG21	1:E:403:THR:HG22	2.02	0.40
1:F:19:LEU:HA	1:F:19:LEU:HD12	1.90	0.40
1:F:44:LEU:HD21	1:F:62:LEU:HD12	2.04	0.40
1:F:327:LYS:HA	1:F:327:LYS:HD3	1.94	0.40
1:G:59:PHE:HZ	1:G:108:ILE:O	2.04	0.40
1:G:151:LEU:HD23	1:G:151:LEU:HA	1.95	0.40
1:G:263:GLN:HB2	1:G:443:ILE:HD12	2.03	0.40
1:J:213:ILE:CD1	1:J:221:LEU:HD13	2.51	0.40
1:J:231:MET:HE1	1:J:256:ALA:CB	2.27	0.40
1:L:473:LYS:HG3	1:L:517:ILE:CG1	2.50	0.40
1:H:320:VAL:HG21	1:H:403:THR:HG22	2.02	0.40
1:A:156:ILE:HA	1:A:162:GLY:O	2.20	0.40
1:A:168:GLY:O	1:A:524:GLN:HA	2.22	0.40
1:C:236:ASP:O	1:C:240:ARG:HG2	2.21	0.40
1:E:242:LYS:HB3	1:E:244:LEU:HD13	2.03	0.40
1:F:236:ASP:O	1:F:240:ARG:HG2	2.21	0.40
1:G:103:ASP:CB	1:G:104:PRO:HD3	2.24	0.40
1:G:357:GLU:OE1	1:G:357:GLU:N	2.54	0.40
1:G:387:ARG:O	1:G:388:GLU:OE1	2.23	0.40
1:I:19:LEU:HD21	1:K:76:GLU:HG3	2.03	0.40
1:I:266:ALA:HB1	1:I:267:PRO:HD2	2.03	0.40
1:J:263:GLN:HE21	1:J:265:LEU:HD21	1.86	0.40
1:J:265:LEU:HA	1:J:289:THR:O	2.20	0.40
1:K:244:LEU:HA	1:K:244:LEU:HD12	1.85	0.40
1:K:597:ARG:CG	1:K:600:GLU:CG	2.92	0.40
1:L:155:PHE:HA	1:L:161:GLY:CA	2.51	0.40
1:L:269:ARG:H	1:L:280:GLN:HG2	1.86	0.40
1:H:91:VAL:HG11	1:L:111:GLN:NE2	2.31	0.40
1:A:175:LYS:NZ	1:A:524:GLN:HA	2.36	0.40
1:A:545:LEU:HD23	1:A:545:LEU:HA	1.86	0.40
1:D:317:LEU:O	1:D:321:ILE:HG13	2.21	0.40
1:E:195:THR:HG23	1:E:203:GLN:NE2	2.36	0.40
1:E:215:ASN:HA	1:E:221:LEU:HD12	2.03	0.40
1:F:263:GLN:NE2	1:F:265:LEU:HD21	2.31	0.40
1:F:466:LEU:HD21	1:F:484:VAL:HG11	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:47:VAL:HG13	1:G:59:PHE:HB2	2.03	0.40
1:G:231:MET:SD	1:G:593:ALA:HA	2.62	0.40
1:G:284:ARG:O	1:G:284:ARG:CG	2.69	0.40
1:G:372:PHE:O	1:G:376:ILE:HG13	2.21	0.40
1:I:215:ASN:HD21	1:I:219:GLU:HA	1.86	0.40
1:I:239:VAL:HG11	1:I:240:ARG:HH21	1.85	0.40
1:I:299:CYS:CB	1:I:332:ALA:HB2	2.52	0.40
1:J:62:LEU:HD23	1:J:63:VAL:O	2.21	0.40
1:J:323:ASN:O	1:J:327:LYS:HG2	2.21	0.40
1:J:406:ALA:CA	1:J:409:ARG:HG2	2.48	0.40
1:K:331:LEU:HD21	1:K:344:VAL:HG12	2.04	0.40
1:K:382:LYS:HE2	1:K:395:TRP:CE2	2.57	0.40
1:L:172:VAL:HG11	1:L:544:ARG:HD2	2.03	0.40
1:L:546:ASP:HB3	1:L:549:GLU:HG2	2.03	0.40

All (8) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:207:ALA:O	1:K:200:GLY:O[1_655]	1.50	0.70
1:A:200:GLY:O	1:D:441:ARG:O[1_655]	1.62	0.58
1:B:285:SER:O	1:E:193:ASP:OD2[3_745]	1.62	0.58
1:B:269:ARG:NH2	1:E:188:ARG:O[3_745]	1.74	0.46
1:B:272:ALA:CB	1:E:250:ALA:O[3_745]	1.88	0.32
1:C:202:ARG:NH1	1:E:261:ASP:OD1[3_745]	1.99	0.21
1:C:202:ARG:NH1	1:E:261:ASP:OD2[3_745]	2.17	0.03
1:J:260:ARG:NH2	1:L:261:ASP:OD1[4_476]	2.17	0.03

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	589/618 (95%)	565 (96%)	24 (4%)	0	100	100
1	B	588/618 (95%)	566 (96%)	22 (4%)	0	100	100
1	C	592/618 (96%)	572 (97%)	20 (3%)	0	100	100
1	D	589/618 (95%)	566 (96%)	23 (4%)	0	100	100
1	E	586/618 (95%)	569 (97%)	17 (3%)	0	100	100
1	F	589/618 (95%)	570 (97%)	19 (3%)	0	100	100
1	G	592/618 (96%)	571 (96%)	21 (4%)	0	100	100
1	H	592/618 (96%)	565 (95%)	27 (5%)	0	100	100
1	I	592/618 (96%)	573 (97%)	19 (3%)	0	100	100
1	J	588/618 (95%)	564 (96%)	24 (4%)	0	100	100
1	K	592/618 (96%)	578 (98%)	14 (2%)	0	100	100
1	L	592/618 (96%)	565 (95%)	27 (5%)	0	100	100
All	All	7081/7416 (96%)	6824 (96%)	257 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	484/499 (97%)	464 (96%)	20 (4%)	27	52
1	B	483/499 (97%)	455 (94%)	28 (6%)	18	45
1	C	485/499 (97%)	470 (97%)	15 (3%)	35	59
1	D	484/499 (97%)	463 (96%)	21 (4%)	26	51
1	E	484/499 (97%)	456 (94%)	28 (6%)	18	45
1	F	484/499 (97%)	468 (97%)	16 (3%)	33	57
1	G	485/499 (97%)	464 (96%)	21 (4%)	26	51
1	H	485/499 (97%)	461 (95%)	24 (5%)	22	49
1	I	485/499 (97%)	440 (91%)	45 (9%)	8	29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	483/499 (97%)	464 (96%)	19 (4%)	28	53
1	K	485/499 (97%)	427 (88%)	58 (12%)	5	19
1	L	485/499 (97%)	453 (93%)	32 (7%)	15	41
All	All	5812/5988 (97%)	5485 (94%)	327 (6%)	19	46

All (327) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	15	ILE
1	H	70	HIS
1	H	91	VAL
1	H	102	VAL
1	H	111	GLN
1	H	147	GLN
1	H	149	LEU
1	H	163	HIS
1	H	219	GLU
1	H	221	LEU
1	H	222	LEU
1	H	350	GLU
1	H	358	ASN
1	H	383	LEU
1	H	386	GLU
1	H	390	GLU
1	H	396	VAL
1	H	397	LEU
1	H	464	VAL
1	H	533	ILE
1	H	561	SER
1	H	569	LEU
1	H	576	VAL
1	H	585	VAL
1	A	15	ILE
1	A	70	HIS
1	A	80	GLU
1	A	86	LEU
1	A	111	GLN
1	A	151	LEU
1	A	163	HIS
1	A	203	GLN
1	A	216	VAL

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Mol	Chain	Res	Type
1	A	223	PHE
1	A	257	GLU
1	A	260	ARG
1	A	364	LEU
1	A	371	THR
1	A	396	VAL
1	A	464	VAL
1	A	576	VAL
1	A	585	VAL
1	A	588	ASN
1	A	601	VAL
1	B	15	ILE
1	B	70	HIS
1	B	83	VAL
1	B	91	VAL
1	B	111	GLN
1	B	163	HIS
1	B	167	SER
1	B	221	LEU
1	B	222	LEU
1	B	223	PHE
1	B	285	SER
1	B	296	ARG
1	B	297	GLU
1	B	324	ILE
1	B	357	GLU
1	B	371	THR
1	B	384	LEU
1	B	388	GLU
1	B	408	THR
1	B	443	ILE
1	B	451	HIS
1	B	464	VAL
1	B	496	GLU
1	B	533	ILE
1	B	561	SER
1	B	569	LEU
1	B	585	VAL
1	B	597	ARG
1	C	15	ILE
1	C	70	HIS
1	C	83	VAL

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Mol	Chain	Res	Type
1	C	91	VAL
1	C	111	GLN
1	C	163	HIS
1	C	223	PHE
1	C	357	GLU
1	C	371	THR
1	C	404	LEU
1	C	439	LEU
1	C	464	VAL
1	C	533	ILE
1	C	561	SER
1	C	585	VAL
1	D	15	ILE
1	D	70	HIS
1	D	82	VAL
1	D	83	VAL
1	D	86	LEU
1	D	91	VAL
1	D	105	GLU
1	D	111	GLN
1	D	163	HIS
1	D	199	SER
1	D	244	LEU
1	D	351	ASP
1	D	354	THR
1	D	398	LYS
1	D	441	ARG
1	D	464	VAL
1	D	533	ILE
1	D	561	SER
1	D	576	VAL
1	D	585	VAL
1	D	601	VAL
1	E	15	ILE
1	E	49	THR
1	E	70	HIS
1	E	82	VAL
1	E	83	VAL
1	E	87	LEU
1	E	102	VAL
1	E	131	ASP
1	E	149	LEU

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Mol	Chain	Res	Type
1	E	163	HIS
1	E	169	ILE
1	E	183	LEU
1	E	195	THR
1	E	223	PHE
1	E	238	VAL
1	E	244	LEU
1	E	262	VAL
1	E	371	THR
1	E	396	VAL
1	E	408	THR
1	E	464	VAL
1	E	524	GLN
1	E	533	ILE
1	E	561	SER
1	E	569	LEU
1	E	576	VAL
1	E	585	VAL
1	E	601	VAL
1	F	15	ILE
1	F	73	VAL
1	F	91	VAL
1	F	102	VAL
1	F	111	GLN
1	F	163	HIS
1	F	199	SER
1	F	282	ASP
1	F	283	GLN
1	F	350	GLU
1	F	388	GLU
1	F	464	VAL
1	F	533	ILE
1	F	561	SER
1	F	576	VAL
1	F	585	VAL
1	G	15	ILE
1	G	70	HIS
1	G	71	GLU
1	G	74	THR
1	G	91	VAL
1	G	102	VAL
1	G	106	ASN

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Mol	Chain	Res	Type
1	G	108	ILE
1	G	164	ILE
1	G	202	ARG
1	G	223	PHE
1	G	232	VAL
1	G	233	GLU
1	G	283	GLN
1	G	350	GLU
1	G	354	THR
1	G	396	VAL
1	G	408	THR
1	G	464	VAL
1	G	533	ILE
1	G	585	VAL
1	I	15	ILE
1	I	24	VAL
1	I	28	VAL
1	I	63	VAL
1	I	70	HIS
1	I	97	VAL
1	I	102	VAL
1	I	111	GLN
1	I	169	ILE
1	I	203	GLN
1	I	206	THR
1	I	217	LYS
1	I	223	PHE
1	I	231	MET
1	I	238	VAL
1	I	244	LEU
1	I	289	THR
1	I	294	THR
1	I	295	ILE
1	I	298	PHE
1	I	317	LEU
1	I	324	ILE
1	I	331	LEU
1	I	336	THR
1	I	349	PHE
1	I	350	GLU
1	I	352	SER
1	I	353	GLU

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Mol	Chain	Res	Type
1	I	355	PRO
1	I	375	LEU
1	I	388	GLU
1	I	390	GLU
1	I	396	VAL
1	I	451	HIS
1	I	464	VAL
1	I	478	ARG
1	I	490	ASN
1	I	504	VAL
1	I	508	ILE
1	I	515	LEU
1	I	561	SER
1	I	576	VAL
1	I	585	VAL
1	I	588	ASN
1	I	604	LEU
1	J	15	ILE
1	J	70	HIS
1	J	79	VAL
1	J	86	LEU
1	J	87	LEU
1	J	91	VAL
1	J	99	VAL
1	J	111	GLN
1	J	219	GLU
1	J	221	LEU
1	J	223	PHE
1	J	244	LEU
1	J	383	LEU
1	J	403	THR
1	J	408	THR
1	J	464	VAL
1	J	533	ILE
1	J	585	VAL
1	J	602	ASP
1	K	15	ILE
1	K	70	HIS
1	K	71	GLU
1	K	86	LEU
1	K	91	VAL
1	K	105	GLU

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Mol	Chain	Res	Type
1	K	106	ASN
1	K	111	GLN
1	K	145	ASP
1	K	149	LEU
1	K	163	HIS
1	K	167	SER
1	K	169	ILE
1	K	176	THR
1	K	191	VAL
1	K	213	ILE
1	K	215	ASN
1	K	219	GLU
1	K	221	LEU
1	K	223	PHE
1	K	244	LEU
1	K	248	ARG
1	K	264	LEU
1	K	277	ILE
1	K	294	THR
1	K	295	ILE
1	K	299	CYS
1	K	304	LEU
1	K	315	LEU
1	K	324	ILE
1	K	325	GLU
1	K	331	LEU
1	K	351	ASP
1	K	357	GLU
1	K	364	LEU
1	K	367	VAL
1	K	371	THR
1	K	385	GLU
1	K	386	GLU
1	K	403	THR
1	K	421	LEU
1	K	426	LEU
1	K	439	LEU
1	K	453	LEU
1	K	456	HIS
1	K	465	LEU
1	K	473	LYS
1	K	480	ASP

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Mol	Chain	Res	Type
1	K	491	LYS
1	K	496	GLU
1	K	501	ILE
1	K	511	ARG
1	K	513	ARG
1	K	533	ILE
1	K	561	SER
1	K	569	LEU
1	K	576	VAL
1	K	585	VAL
1	L	15	ILE
1	L	27	THR
1	L	39	VAL
1	L	49	THR
1	L	70	HIS
1	L	75	PHE
1	L	77	SER
1	L	86	LEU
1	L	91	VAL
1	L	131	ASP
1	L	145	ASP
1	L	149	LEU
1	L	221	LEU
1	L	223	PHE
1	L	244	LEU
1	L	317	LEU
1	L	359	LEU
1	L	371	THR
1	L	383	LEU
1	L	397	LEU
1	L	408	THR
1	L	414	VAL
1	L	464	VAL
1	L	468	GLU
1	L	476	VAL
1	L	489	LEU
1	L	533	ILE
1	L	561	SER
1	L	576	VAL
1	L	585	VAL
1	L	588	ASN
1	L	603	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (69) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	106	ASN
1	H	147	GLN
1	H	228	ASN
1	H	263	GLN
1	H	415	GLN
1	H	583	ASN
1	H	588	ASN
1	A	163	HIS
1	A	228	ASN
1	A	263	GLN
1	A	444	GLN
1	B	115	HIS
1	B	228	ASN
1	B	263	GLN
1	B	444	GLN
1	B	451	HIS
1	B	523	GLN
1	C	106	ASN
1	C	263	GLN
1	C	368	ASN
1	C	523	GLN
1	D	115	HIS
1	D	163	HIS
1	D	228	ASN
1	D	263	GLN
1	D	283	GLN
1	D	399	GLN
1	D	451	HIS
1	E	163	HIS
1	E	184	HIS
1	E	203	GLN
1	E	263	GLN
1	E	444	GLN
1	F	106	ASN
1	F	163	HIS
1	F	165	ASN
1	F	203	GLN
1	F	263	GLN
1	F	345	HIS
1	F	444	GLN
1	G	263	GLN

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Mol	Chain	Res	Type
1	G	283	GLN
1	G	523	GLN
1	G	588	ASN
1	I	70	HIS
1	I	106	ASN
1	I	111	GLN
1	I	147	GLN
1	I	184	HIS
1	I	228	ASN
1	I	263	GLN
1	I	280	GLN
1	I	323	ASN
1	I	430	GLN
1	I	451	HIS
1	I	588	ASN
1	J	70	HIS
1	J	197	GLN
1	J	263	GLN
1	J	283	GLN
1	K	358	ASN
1	K	368	ASN
1	K	451	HIS
1	K	456	HIS
1	L	70	HIS
1	L	111	GLN
1	L	115	HIS
1	L	165	ASN
1	L	583	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 14 ligands modelled in this entry, 2 are monoatomic - leaving 12 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
3	ADP	B	1001	-	28,29,29	0.73	2 (7%)	43,45,45	0.75	1 (2%)
3	ADP	C	1001	-	28,29,29	0.84	1 (3%)	43,45,45	0.75	1 (2%)
3	ADP	K	1001	-	28,29,29	0.93	3 (10%)	43,45,45	0.85	2 (4%)
3	ADP	G	1001	-	28,29,29	0.80	1 (3%)	43,45,45	0.81	1 (2%)
3	ADP	F	1001	-	28,29,29	0.71	0	43,45,45	0.83	2 (4%)
3	ADP	D	1001	2	28,29,29	0.78	0	43,45,45	0.85	2 (4%)
3	ADP	J	1001	-	28,29,29	0.78	1 (3%)	43,45,45	0.69	0
3	ADP	L	1001	-	28,29,29	0.85	3 (10%)	43,45,45	0.68	0
3	ADP	A	1001	-	28,29,29	0.79	1 (3%)	43,45,45	0.77	1 (2%)
3	ADP	E	1001	-	28,29,29	0.74	1 (3%)	43,45,45	0.74	0
3	ADP	H	1001	2	28,29,29	0.87	2 (7%)	43,45,45	0.86	2 (4%)
3	ADP	I	1001	-	28,29,29	0.83	1 (3%)	43,45,45	0.82	1 (2%)

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
3	ADP	B	1001	-	-	9/16/32/32	0/3/3/3
3	ADP	C	1001	-	-	4/16/32/32	0/3/3/3
3	ADP	K	1001	-	-	7/16/32/32	0/3/3/3
3	ADP	G	1001	-	-	8/16/32/32	0/3/3/3
3	ADP	F	1001	-	-	7/16/32/32	0/3/3/3
3	ADP	D	1001	2	-	6/16/32/32	0/3/3/3
3	ADP	J	1001	-	-	5/16/32/32	0/3/3/3
3	ADP	L	1001	-	-	6/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	A	1001	-	-	6/16/32/32	0/3/3/3
3	ADP	E	1001	-	-	7/16/32/32	0/3/3/3
3	ADP	H	1001	2	-	8/16/32/32	0/3/3/3
3	ADP	I	1001	-	-	8/16/32/32	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	1001	ADP	PB-O2B	-2.54	1.45	1.54
3	E	1001	ADP	PA-O3A	-2.45	1.56	1.59
3	L	1001	ADP	PB-O3B	-2.30	1.46	1.54
3	K	1001	ADP	PA-O3A	-2.29	1.57	1.59
3	G	1001	ADP	PB-O2B	-2.29	1.46	1.54
3	H	1001	ADP	PB-O2B	-2.29	1.46	1.54
3	C	1001	ADP	PB-O2B	-2.26	1.46	1.54
3	B	1001	ADP	PB-O3B	-2.22	1.46	1.54
3	I	1001	ADP	PB-O3B	-2.21	1.46	1.54
3	A	1001	ADP	PB-O2B	-2.18	1.46	1.54
3	J	1001	ADP	PB-O3B	-2.13	1.46	1.54
3	L	1001	ADP	PA-O3A	-2.08	1.57	1.59
3	H	1001	ADP	PB-O3B	-2.07	1.47	1.54
3	K	1001	ADP	PB-O3B	-2.03	1.47	1.54
3	B	1001	ADP	PB-O2B	-2.01	1.47	1.54
3	L	1001	ADP	PB-O2B	-2.01	1.47	1.54

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1001	ADP	C2'-C3'-C4'	-2.74	97.32	102.61
3	K	1001	ADP	O3'-C3'-C2'	-2.53	103.71	111.82
3	B	1001	ADP	O3'-C3'-C2'	-2.49	103.83	111.82
3	K	1001	ADP	O4'-C4'-C3'	-2.48	100.22	105.15
3	H	1001	ADP	C2'-C3'-C4'	-2.30	98.16	102.61
3	G	1001	ADP	O3'-C3'-C2'	-2.25	104.59	111.82
3	H	1001	ADP	O4'-C4'-C3'	-2.23	100.73	105.15
3	D	1001	ADP	O4'-C4'-C3'	-2.22	100.75	105.15
3	C	1001	ADP	C2'-C3'-C4'	-2.15	98.46	102.61
3	F	1001	ADP	O4'-C4'-C3'	-2.11	100.96	105.15
3	A	1001	ADP	O4'-C4'-C3'	-2.02	101.15	105.15
3	I	1001	ADP	C2'-C3'-C4'	-2.01	98.73	102.61
3	F	1001	ADP	C2'-C3'-C4'	-2.00	98.74	102.61

There are no chirality outliers.

All (81) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	H	1001	ADP	C2'-C1'-N9-C8
3	C	1001	ADP	C2'-C1'-N9-C8
3	F	1001	ADP	C5'-O5'-PA-O2A
3	F	1001	ADP	C5'-O5'-PA-O3A
3	F	1001	ADP	C2'-C1'-N9-C8
3	F	1001	ADP	C2'-C1'-N9-C4
3	G	1001	ADP	C5'-O5'-PA-O3A
3	G	1001	ADP	C2'-C1'-N9-C8
3	I	1001	ADP	C5'-O5'-PA-O1A
3	K	1001	ADP	C5'-O5'-PA-O2A
3	K	1001	ADP	C2'-C1'-N9-C8
3	K	1001	ADP	C2'-C1'-N9-C4
3	L	1001	ADP	C5'-O5'-PA-O1A
3	L	1001	ADP	C2'-C1'-N9-C8
3	H	1001	ADP	C2'-C1'-N9-C4
3	C	1001	ADP	C2'-C1'-N9-C4
3	G	1001	ADP	C2'-C1'-N9-C4
3	L	1001	ADP	C2'-C1'-N9-C4
3	H	1001	ADP	C3'-C4'-C5'-O5'
3	A	1001	ADP	C3'-C4'-C5'-O5'
3	C	1001	ADP	C3'-C4'-C5'-O5'
3	E	1001	ADP	C3'-C4'-C5'-O5'
3	H	1001	ADP	O4'-C4'-C5'-O5'
3	C	1001	ADP	O4'-C4'-C5'-O5'
3	E	1001	ADP	O4'-C4'-C5'-O5'
3	F	1001	ADP	O4'-C4'-C5'-O5'
3	F	1001	ADP	C3'-C4'-C5'-O5'
3	A	1001	ADP	C2'-C1'-N9-C8
3	B	1001	ADP	C2'-C1'-N9-C8
3	J	1001	ADP	C2'-C1'-N9-C8
3	I	1001	ADP	C3'-C4'-C5'-O5'
3	K	1001	ADP	C3'-C4'-C5'-O5'
3	A	1001	ADP	O4'-C4'-C5'-O5'
3	D	1001	ADP	O4'-C4'-C5'-O5'
3	D	1001	ADP	C3'-C4'-C5'-O5'
3	I	1001	ADP	C2'-C1'-N9-C8
3	B	1001	ADP	C3'-C4'-C5'-O5'
3	I	1001	ADP	O4'-C4'-C5'-O5'
3	I	1001	ADP	PB-O3A-PA-O1A
3	K	1001	ADP	O4'-C4'-C5'-O5'

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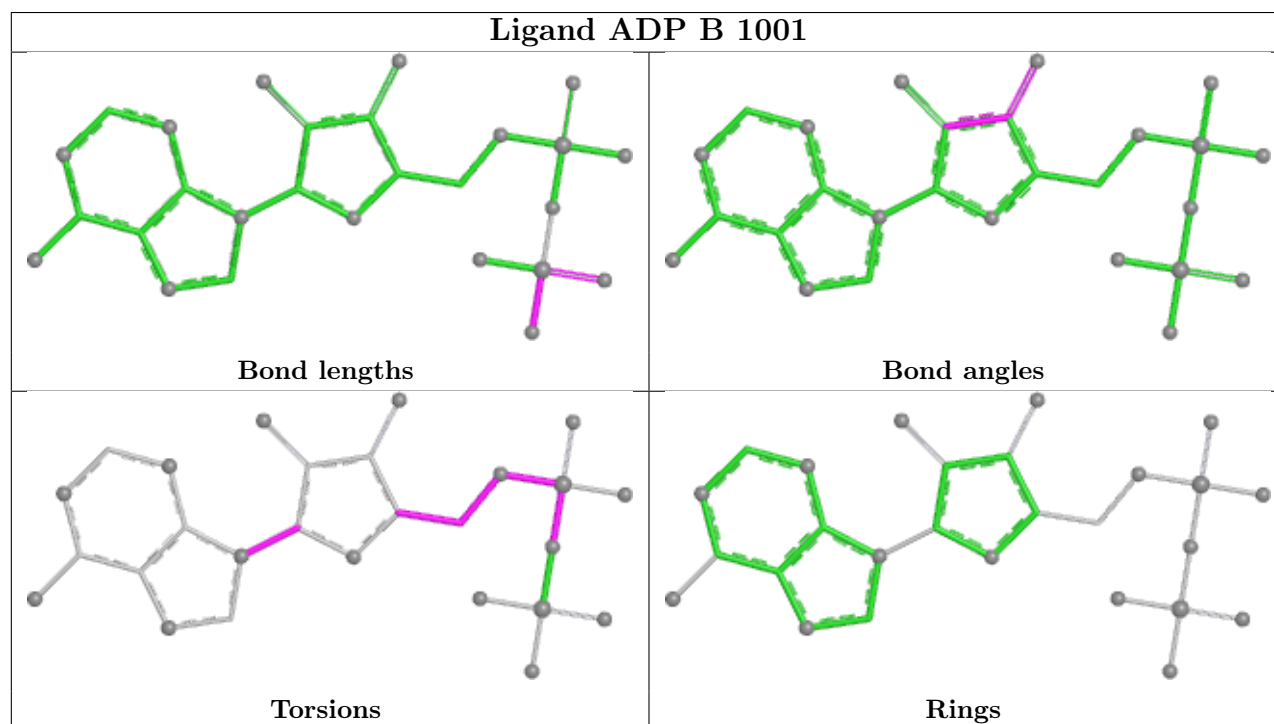
Mol	Chain	Res	Type	Atoms
3	J	1001	ADP	C2'-C1'-N9-C4
3	A	1001	ADP	C4'-C5'-O5'-PA
3	J	1001	ADP	C3'-C4'-C5'-O5'
3	B	1001	ADP	PB-O3A-PA-O5'
3	E	1001	ADP	C2'-C1'-N9-C8
3	B	1001	ADP	O4'-C4'-C5'-O5'
3	D	1001	ADP	C2'-C1'-N9-C8
3	B	1001	ADP	PB-O3A-PA-O1A
3	G	1001	ADP	PB-O3A-PA-O1A
3	G	1001	ADP	C3'-C4'-C5'-O5'
3	J	1001	ADP	C4'-C5'-O5'-PA
3	K	1001	ADP	C4'-C5'-O5'-PA
3	A	1001	ADP	C2'-C1'-N9-C4
3	B	1001	ADP	C5'-O5'-PA-O1A
3	D	1001	ADP	C5'-O5'-PA-O1A
3	G	1001	ADP	C5'-O5'-PA-O1A
3	K	1001	ADP	C5'-O5'-PA-O3A
3	L	1001	ADP	C5'-O5'-PA-O3A
3	B	1001	ADP	C4'-C5'-O5'-PA
3	F	1001	ADP	C4'-C5'-O5'-PA
3	H	1001	ADP	PB-O3A-PA-O1A
3	I	1001	ADP	PB-O3A-PA-O2A
3	B	1001	ADP	C2'-C1'-N9-C4
3	E	1001	ADP	C2'-C1'-N9-C4
3	I	1001	ADP	C2'-C1'-N9-C4
3	J	1001	ADP	O4'-C4'-C5'-O5'
3	H	1001	ADP	PB-O3A-PA-O2A
3	L	1001	ADP	PB-O3A-PA-O2A
3	D	1001	ADP	O4'-C1'-N9-C8
3	H	1001	ADP	PA-O3A-PB-O2B
3	H	1001	ADP	PA-O3A-PB-O3B
3	L	1001	ADP	PA-O3A-PB-O2B
3	G	1001	ADP	O4'-C4'-C5'-O5'
3	E	1001	ADP	O4'-C1'-N9-C8
3	E	1001	ADP	PB-O3A-PA-O1A
3	E	1001	ADP	PB-O3A-PA-O2A
3	G	1001	ADP	PB-O3A-PA-O2A
3	A	1001	ADP	O4'-C1'-N9-C8
3	D	1001	ADP	C2'-C1'-N9-C4
3	I	1001	ADP	O4'-C1'-N9-C8
3	B	1001	ADP	O4'-C1'-N9-C8

There are no ring outliers.

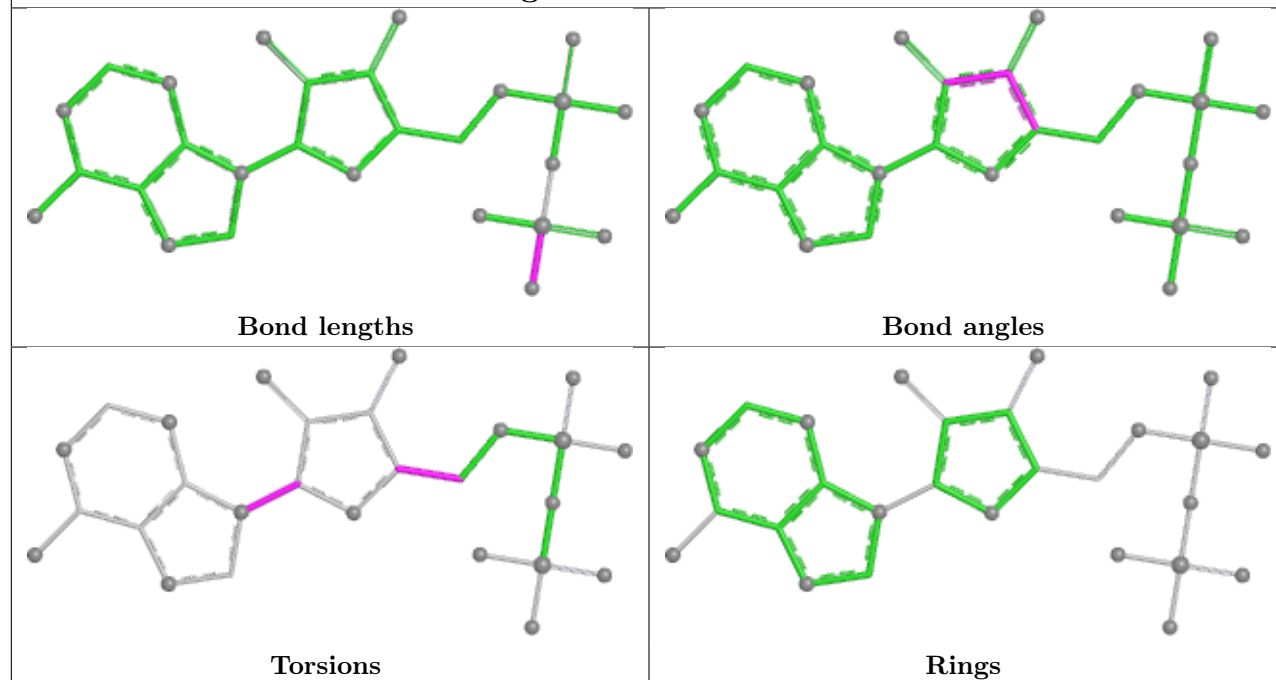
11 monomers are involved in 53 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1001	ADP	6	0
3	C	1001	ADP	3	0
3	K	1001	ADP	6	0
3	G	1001	ADP	2	0
3	F	1001	ADP	3	0
3	D	1001	ADP	3	0
3	J	1001	ADP	4	0
3	L	1001	ADP	1	0
3	A	1001	ADP	9	0
3	E	1001	ADP	15	0
3	H	1001	ADP	1	0

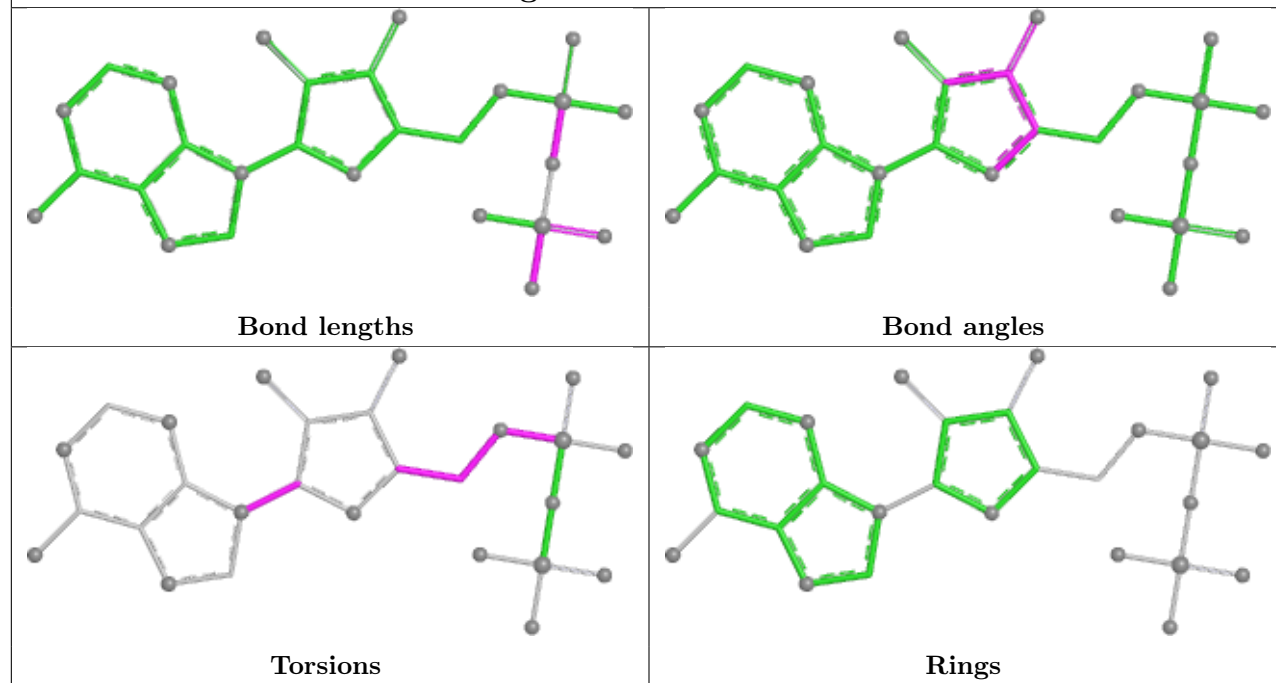
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



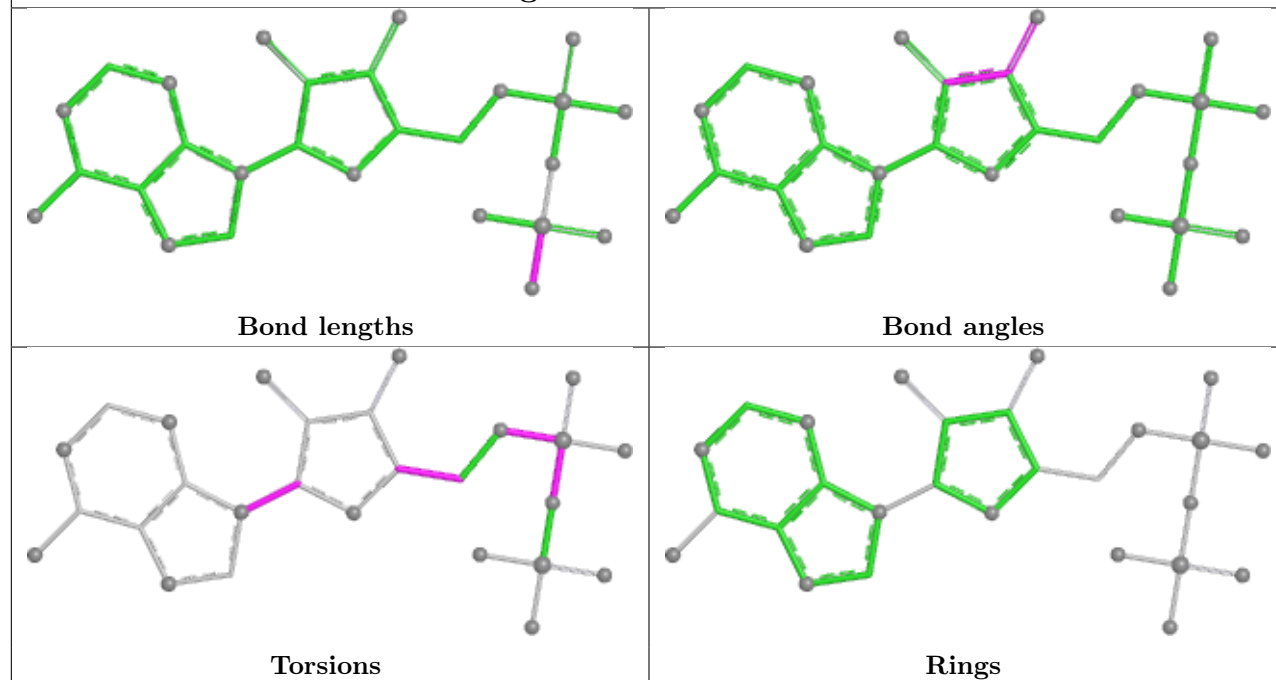
Ligand ADP C 1001



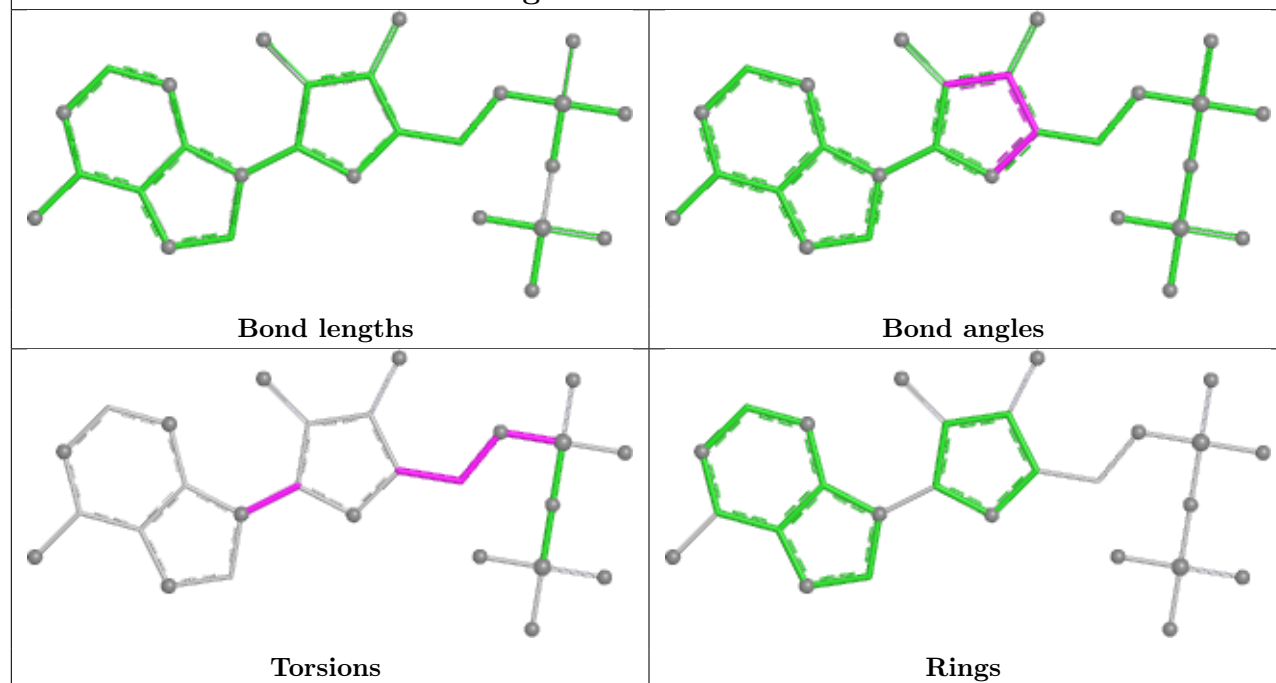
Ligand ADP K 1001



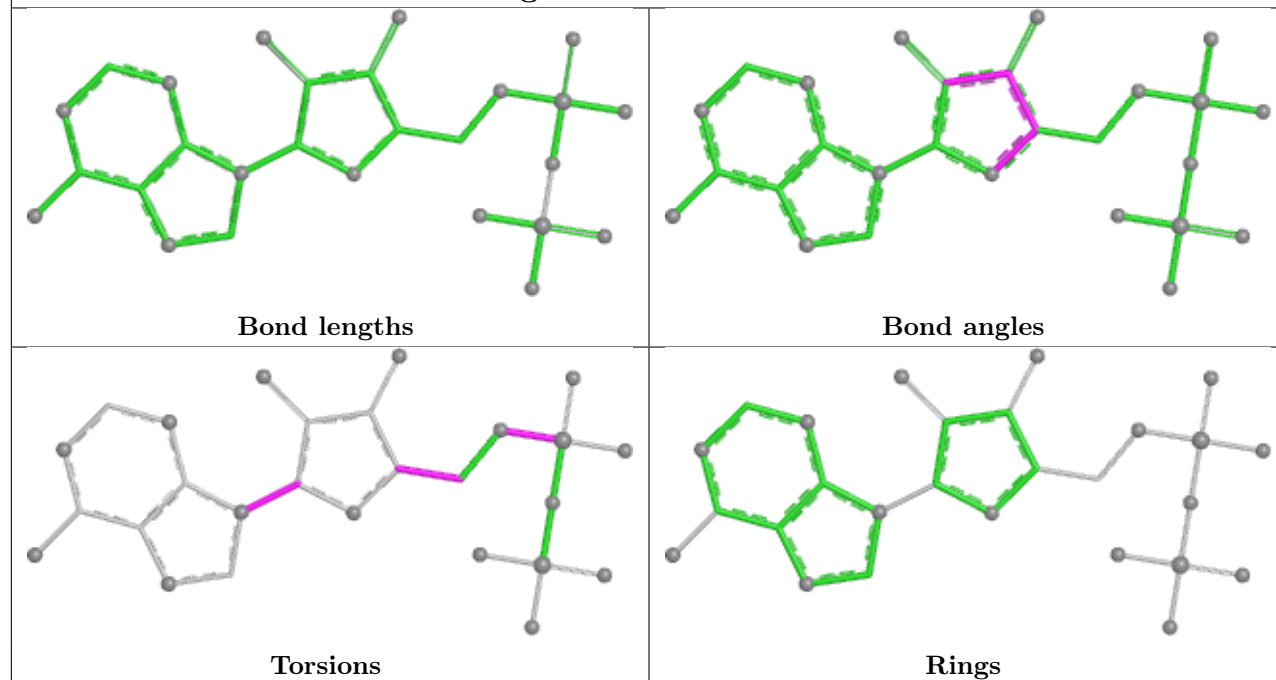
Ligand ADP G 1001



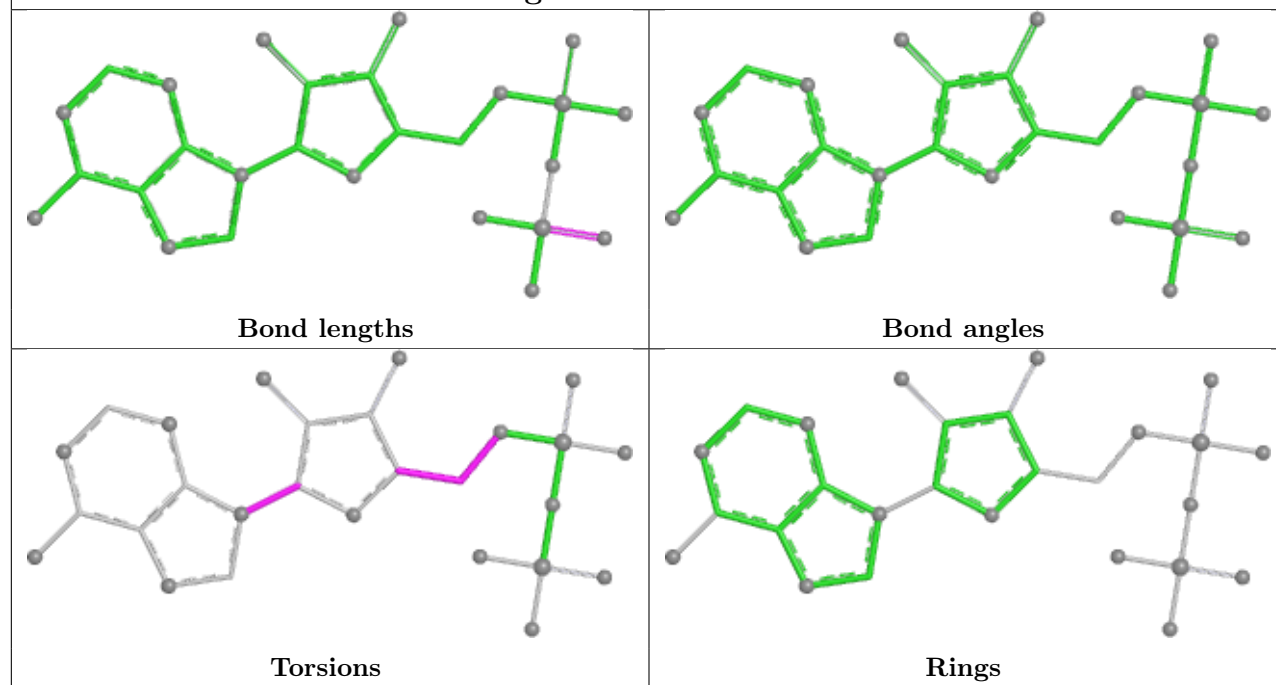
Ligand ADP F 1001



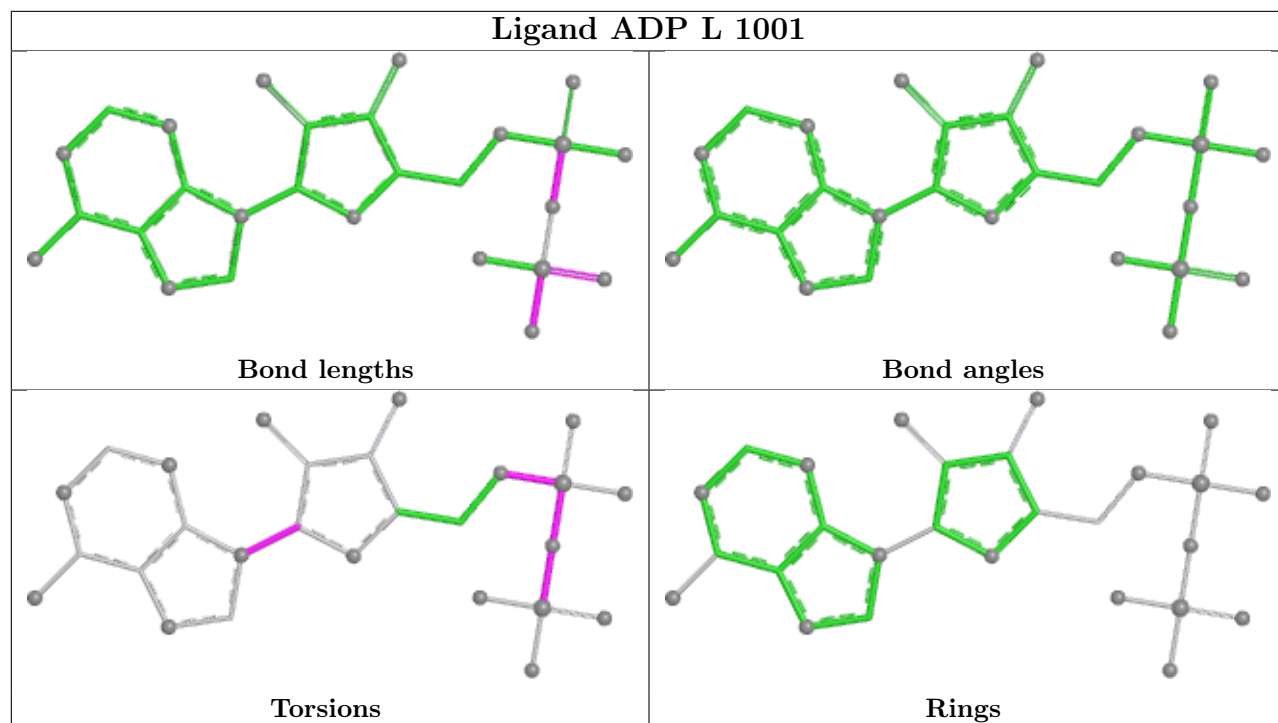
Ligand ADP D 1001



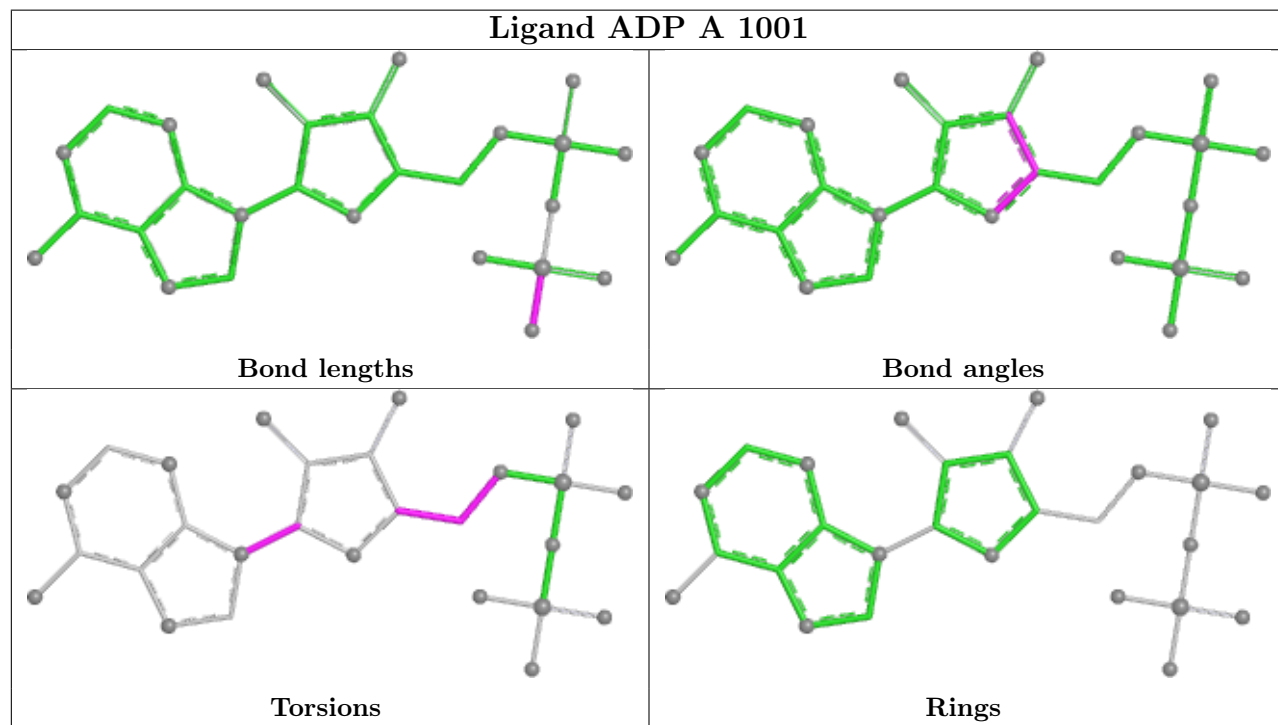
Ligand ADP J 1001



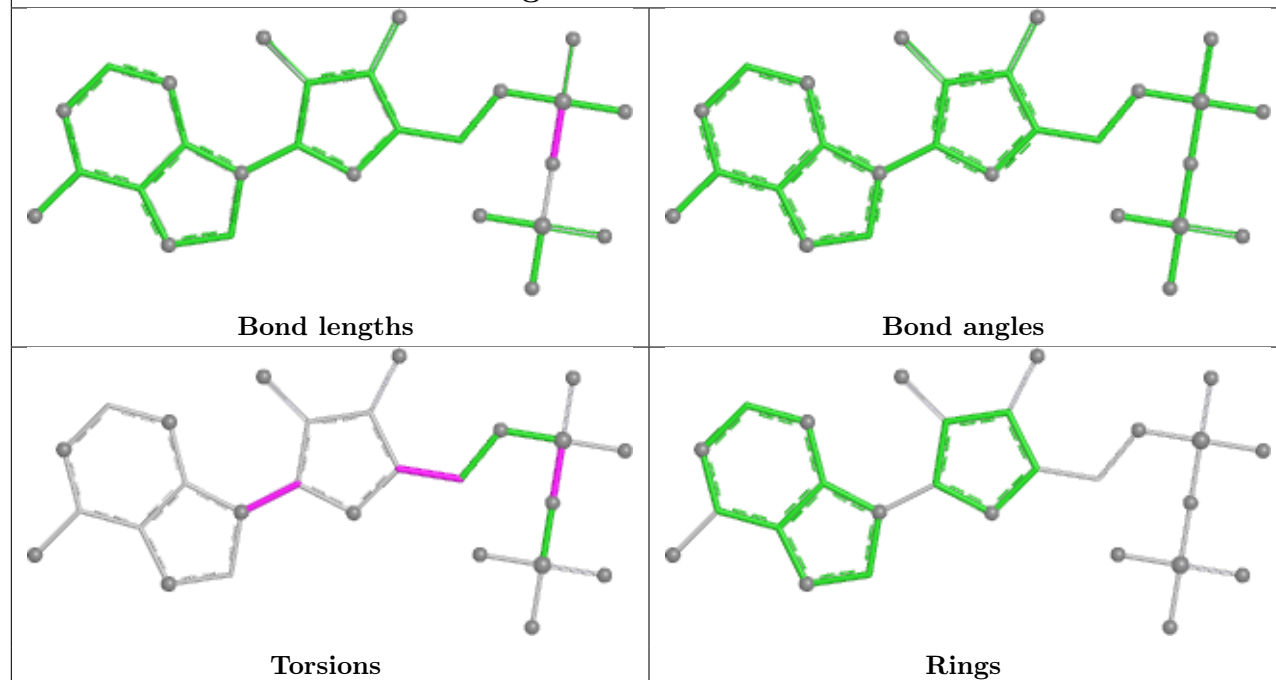
Ligand ADP L 1001



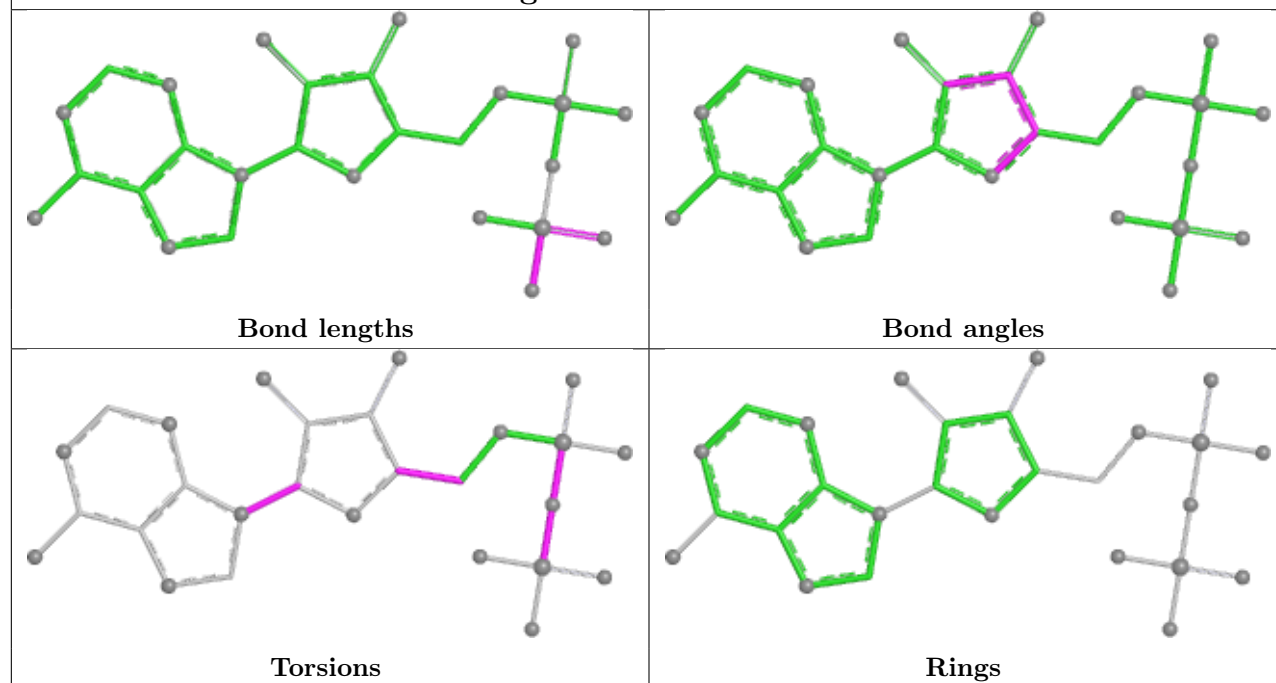
Ligand ADP A 1001

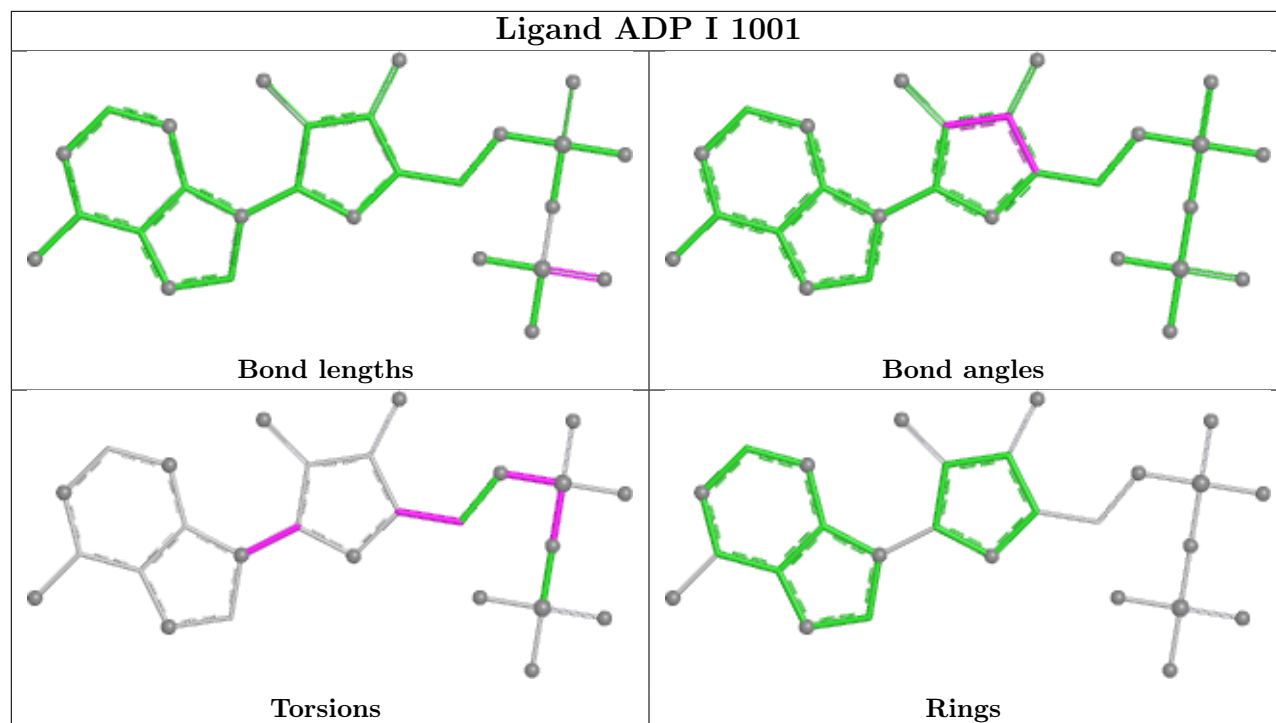


Ligand ADP E 1001



Ligand ADP H 1001





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	A	591/618 (95%)	0.27	28 (4%)	36	27	55, 65, 78, 88	0
1	B	590/618 (95%)	0.26	26 (4%)	39	28	55, 66, 79, 89	0
1	C	594/618 (96%)	0.32	27 (4%)	38	28	57, 70, 81, 90	0
1	D	591/618 (95%)	0.31	25 (4%)	40	29	63, 76, 85, 92	0
1	E	590/618 (95%)	0.28	16 (2%)	56	42	62, 73, 83, 91	0
1	F	591/618 (95%)	0.20	22 (3%)	45	32	58, 68, 79, 87	0
1	G	594/618 (96%)	0.27	27 (4%)	38	28	55, 65, 76, 85	0
1	H	594/618 (96%)	0.36	29 (4%)	35	26	52, 64, 76, 86	0
1	I	594/618 (96%)	0.11	15 (2%)	58	43	57, 68, 81, 87	0
1	J	590/618 (95%)	0.38	28 (4%)	36	27	64, 74, 86, 94	0
1	K	594/618 (96%)	0.18	15 (2%)	58	43	60, 71, 83, 90	0
1	L	594/618 (96%)	0.48	29 (4%)	35	26	59, 71, 82, 93	0
All	All	7107/7416 (95%)	0.28	287 (4%)	42	30	52, 70, 82, 94	0

All (287) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	312	SER	7.5
1	I	312	SER	7.1
1	J	313	ALA	6.0
1	D	311	ALA	5.9
1	J	476	VAL	5.3
1	B	313	ALA	5.2
1	G	312	SER	5.0
1	L	313	ALA	5.0
1	G	311	ALA	4.9
1	A	313	ALA	4.9
1	A	476	VAL	4.6

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Mol	Chain	Res	Type	RSRZ
1	E	309	SER	4.5
1	F	309	SER	4.5
1	L	312	SER	4.5
1	G	356	PRO	4.5
1	H	564	GLY	4.5
1	J	131	ASP	4.4
1	L	162	GLY	4.4
1	H	313	ALA	4.3
1	G	276	ALA	4.1
1	D	313	ALA	4.1
1	F	312	SER	4.0
1	I	311	ALA	4.0
1	F	203	GLN	4.0
1	E	275	THR	3.9
1	F	205	GLY	3.9
1	L	356	PRO	3.9
1	H	223	PHE	3.8
1	D	276	ALA	3.7
1	H	312	SER	3.7
1	L	373	GLU	3.7
1	E	312	SER	3.7
1	F	480	ASP	3.6
1	I	313	ALA	3.6
1	B	200	GLY	3.6
1	F	313	ALA	3.5
1	C	269	ARG	3.5
1	H	415	GLN	3.5
1	B	351	ASP	3.5
1	B	204	SER	3.5
1	J	311	ALA	3.5
1	L	272	ALA	3.5
1	C	323	ASN	3.4
1	C	272	ALA	3.4
1	L	425	ASP	3.4
1	H	350	GLU	3.4
1	I	272	ALA	3.4
1	E	271	GLY	3.4
1	C	312	SER	3.3
1	H	273	ALA	3.3
1	C	145	ASP	3.3
1	B	203	GLN	3.3
1	J	273	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	472	TYR	3.3
1	A	311	ALA	3.3
1	E	313	ALA	3.3
1	F	311	ALA	3.3
1	B	198	GLY	3.3
1	K	274	GLY	3.2
1	C	355	PRO	3.2
1	G	351	ASP	3.2
1	H	203	GLN	3.2
1	A	270	ALA	3.2
1	B	318	GLY	3.1
1	D	318	GLY	3.1
1	G	208	GLY	3.1
1	H	386	GLU	3.1
1	E	203	GLN	3.1
1	J	274	GLY	3.1
1	H	385	GLU	3.1
1	A	480	ASP	3.1
1	B	311	ALA	3.0
1	K	358	ASN	3.0
1	L	358	ASN	3.0
1	A	312	SER	3.0
1	K	312	SER	3.0
1	D	355	PRO	3.0
1	F	270	ALA	3.0
1	C	310	ASP	3.0
1	L	391	GLY	3.0
1	A	310	ASP	3.0
1	G	225	ASP	3.0
1	G	480	ASP	3.0
1	F	260	ARG	3.0
1	G	204	SER	3.0
1	E	479	GLN	3.0
1	H	311	ALA	2.9
1	G	270	ALA	2.9
1	L	476	VAL	2.9
1	A	366	GLY	2.9
1	H	348	GLN	2.9
1	L	275	THR	2.9
1	H	417	TYR	2.9
1	E	314	SER	2.9
1	F	271	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	J	391	GLY	2.9
1	H	104	PRO	2.9
1	A	332	ALA	2.9
1	J	120	ALA	2.9
1	C	313	ALA	2.8
1	F	351	ASP	2.8
1	C	158	GLY	2.8
1	J	312	SER	2.8
1	A	276	ALA	2.8
1	G	313	ALA	2.8
1	H	225	ASP	2.8
1	C	311	ALA	2.8
1	G	273	ALA	2.8
1	G	350	GLU	2.8
1	H	356	PRO	2.8
1	G	314	SER	2.8
1	E	162	GLY	2.7
1	G	310	ASP	2.7
1	K	323	ASN	2.7
1	D	314	SER	2.7
1	J	385	GLU	2.7
1	J	456	HIS	2.7
1	I	356	PRO	2.7
1	I	281	THR	2.7
1	H	270	ALA	2.7
1	J	269	ARG	2.7
1	H	351	ASP	2.7
1	E	593	ALA	2.7
1	L	152	ASN	2.7
1	B	356	PRO	2.7
1	L	605	GLY	2.7
1	B	207	ALA	2.7
1	B	309	SER	2.6
1	F	204	SER	2.6
1	I	207	ALA	2.6
1	B	352	SER	2.6
1	A	286	GLU	2.6
1	J	427	THR	2.6
1	B	314	SER	2.6
1	K	356	PRO	2.6
1	J	233	GLU	2.6
1	G	269	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	H	199	SER	2.5
1	C	309	SER	2.5
1	F	285	SER	2.5
1	A	271	GLY	2.5
1	G	318	GLY	2.5
1	B	480	ASP	2.5
1	C	103	ASP	2.5
1	C	351	ASP	2.5
1	E	311	ALA	2.5
1	I	208	GLY	2.5
1	I	479	GLN	2.5
1	H	80	GLU	2.5
1	J	373	GLU	2.5
1	L	355	PRO	2.5
1	D	312	SER	2.5
1	C	120	ALA	2.5
1	B	490	ASN	2.5
1	D	316	ASN	2.5
1	L	351	ASP	2.5
1	A	240	ARG	2.4
1	F	198	GLY	2.4
1	J	433	GLY	2.4
1	K	201	GLY	2.4
1	K	271	GLY	2.4
1	C	430	GLN	2.4
1	F	272	ALA	2.4
1	L	350	GLU	2.4
1	L	428	PRO	2.4
1	F	208	GLY	2.4
1	A	120	ALA	2.4
1	G	231	MET	2.4
1	A	475	ARG	2.4
1	A	531	ARG	2.4
1	E	177	SER	2.4
1	J	309	SER	2.4
1	C	275	THR	2.4
1	E	480	ASP	2.4
1	K	103	ASP	2.4
1	K	120	ALA	2.4
1	K	270	ALA	2.4
1	G	385	GLU	2.4
1	D	275	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	103	ASP	2.4
1	B	389	GLY	2.4
1	B	413	GLY	2.4
1	C	389	GLY	2.4
1	I	225	ASP	2.3
1	J	430	GLN	2.3
1	B	357	GLU	2.3
1	J	285	SER	2.3
1	J	198	GLY	2.3
1	L	206	THR	2.3
1	C	456	HIS	2.3
1	D	144	ALA	2.3
1	H	381	TYR	2.3
1	D	381	TYR	2.3
1	K	310	ASP	2.3
1	A	356	PRO	2.3
1	D	274	GLY	2.3
1	D	366	GLY	2.3
1	H	272	ALA	2.3
1	A	275	THR	2.3
1	K	145	ASP	2.3
1	B	468	GLU	2.3
1	C	85	GLY	2.3
1	I	595	ALA	2.3
1	B	206	THR	2.3
1	C	90	SER	2.3
1	D	352	SER	2.3
1	G	199	SER	2.3
1	G	525	THR	2.3
1	A	203	GLN	2.3
1	B	363	GLU	2.3
1	D	356	PRO	2.3
1	E	355	PRO	2.3
1	H	595	ALA	2.3
1	C	477	GLY	2.3
1	F	455	ALA	2.3
1	A	309	SER	2.3
1	L	536	ASN	2.3
1	D	357	GLU	2.2
1	L	357	GLU	2.2
1	J	567	GLY	2.2
1	L	49	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	K	309	SER	2.2
1	H	430	GLN	2.2
1	D	358	ASN	2.2
1	F	316	ASN	2.2
1	J	270	ALA	2.2
1	K	605	GLY	2.2
1	L	564	GLY	2.2
1	D	203	GLN	2.2
1	F	114	ASP	2.2
1	L	225	ASP	2.2
1	K	273	ALA	2.2
1	H	74	THR	2.2
1	C	314	SER	2.2
1	A	273	ALA	2.2
1	A	599	ASP	2.2
1	D	603	ASP	2.2
1	J	381	TYR	2.2
1	C	204	SER	2.2
1	I	276	ALA	2.2
1	L	37	ALA	2.2
1	H	240	ARG	2.2
1	A	430	GLN	2.1
1	D	373	GLU	2.1
1	H	274	GLY	2.1
1	F	190	GLY	2.1
1	J	200	GLY	2.1
1	A	145	ASP	2.1
1	D	537	ALA	2.1
1	I	240	ARG	2.1
1	I	593	ALA	2.1
1	H	454	SER	2.1
1	C	318	GLY	2.1
1	G	218	GLY	2.1
1	J	161	GLY	2.1
1	J	310	ASP	2.1
1	A	281	THR	2.1
1	B	202	ARG	2.1
1	G	233	GLU	2.1
1	I	99	VAL	2.1
1	D	451	HIS	2.1
1	C	273	ALA	2.1
1	C	276	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	272	ALA	2.1
1	B	243	GLY	2.1
1	G	200	GLY	2.1
1	B	355	PRO	2.1
1	C	356	PRO	2.1
1	L	432	GLU	2.1
1	A	314	SER	2.1
1	E	199	SER	2.1
1	F	323	ASN	2.1
1	D	310	ASP	2.1
1	J	472	TYR	2.1
1	D	219	GLU	2.1
1	L	123	GLU	2.1
1	L	604	LEU	2.0
1	G	427	THR	2.0
1	L	381	TYR	2.0
1	D	88	PRO	2.0
1	E	185	SER	2.0
1	B	358	ASN	2.0
1	H	250	ALA	2.0
1	J	425	ASP	2.0
1	L	271	GLY	2.0
1	F	356	PRO	2.0
1	G	429	GLU	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 [i](#)

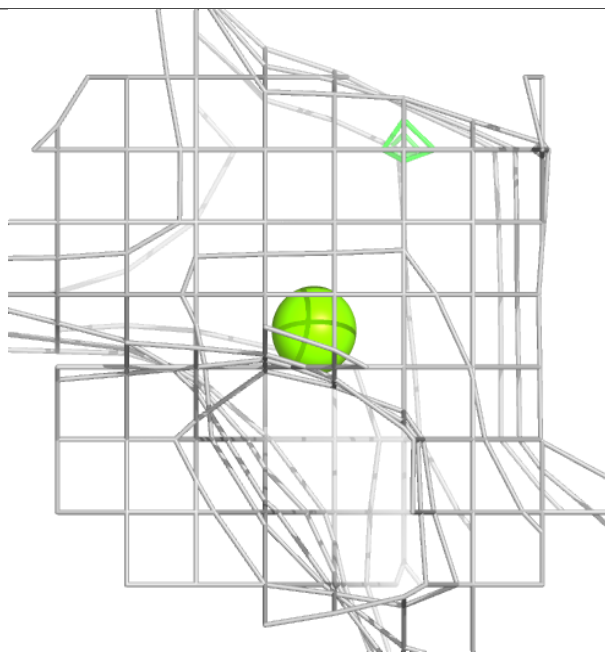
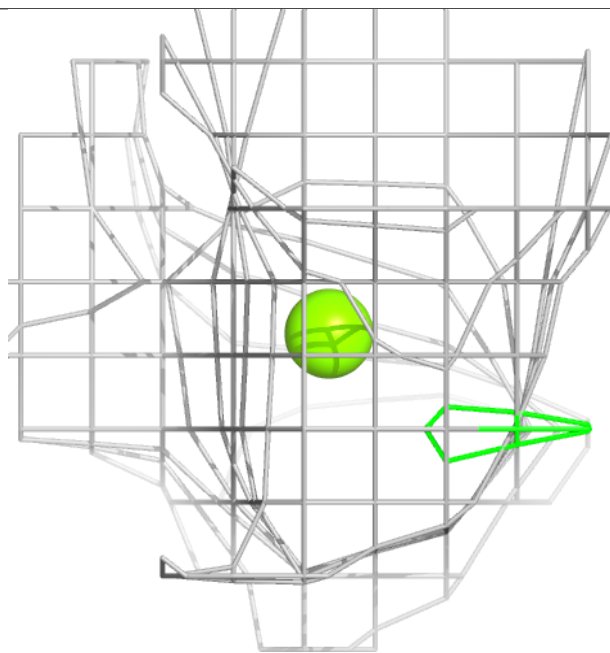
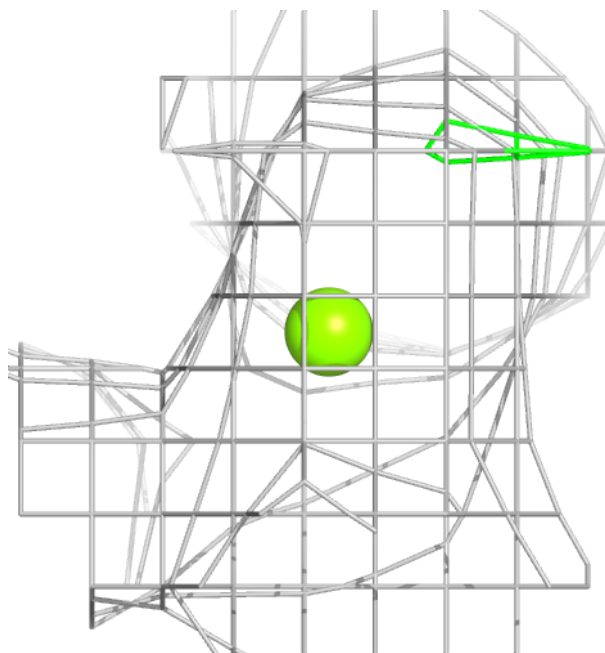
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MG	D	1000	1/1	0.71	0.13	71,71,71,71	0
3	ADP	E	1001	27/27	0.76	0.18	71,72,72,73	0
3	ADP	F	1001	27/27	0.84	0.12	65,65,66,66	0
3	ADP	D	1001	27/27	0.86	0.10	74,75,75,75	0
3	ADP	B	1001	27/27	0.88	0.10	65,66,67,67	0
3	ADP	L	1001	27/27	0.89	0.10	70,71,71,71	0
3	ADP	K	1001	27/27	0.90	0.09	66,67,68,68	0
3	ADP	G	1001	27/27	0.90	0.10	62,63,63,64	0
3	ADP	J	1001	27/27	0.92	0.08	70,70,71,71	0
3	ADP	C	1001	27/27	0.92	0.08	70,71,71,71	0
3	ADP	I	1001	27/27	0.92	0.10	66,66,67,67	0
3	ADP	A	1001	27/27	0.93	0.09	64,65,65,65	0
3	ADP	H	1001	27/27	0.94	0.07	62,64,65,65	0
2	MG	H	1000	1/1	0.94	0.12	65,65,65,65	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.

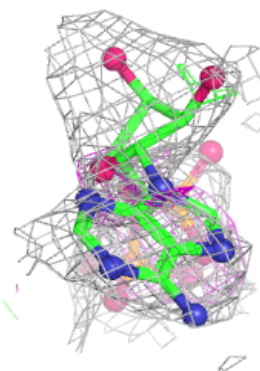
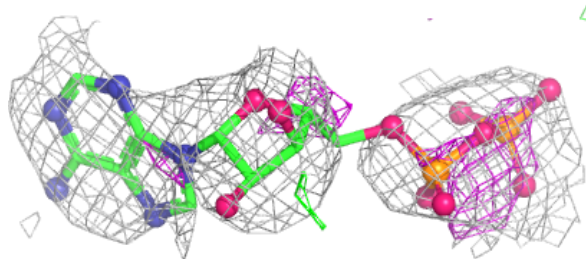
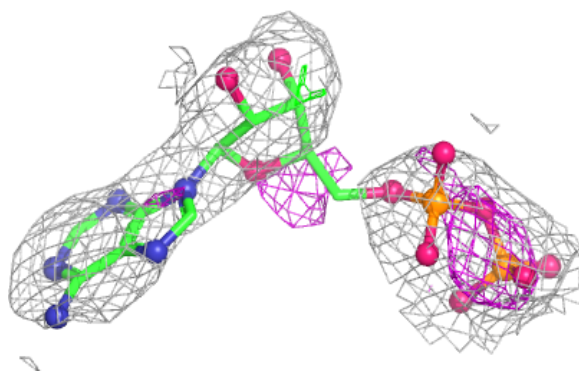
Electron density around MG D 1000:

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

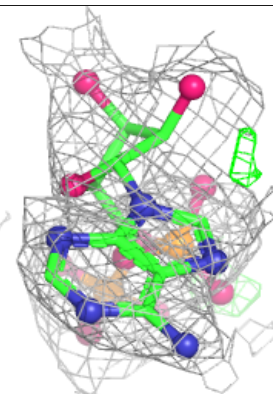
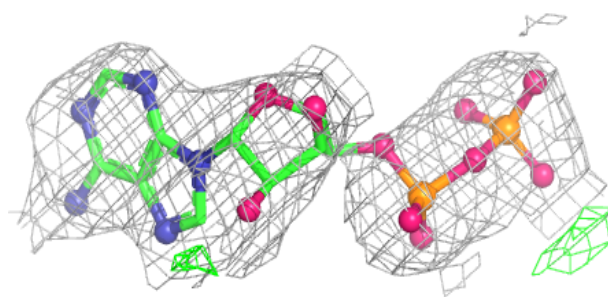
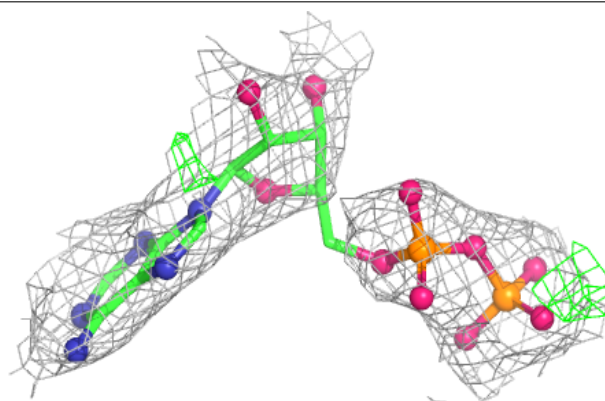


Electron density around ADP E 1001:

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

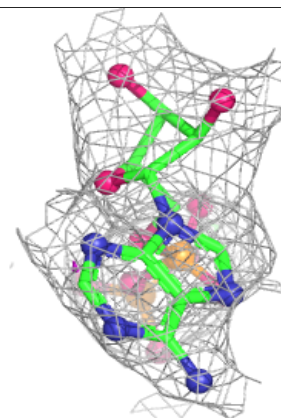
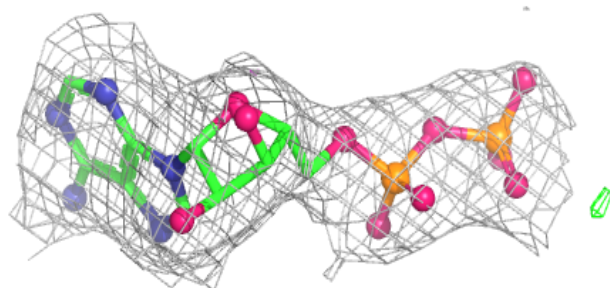
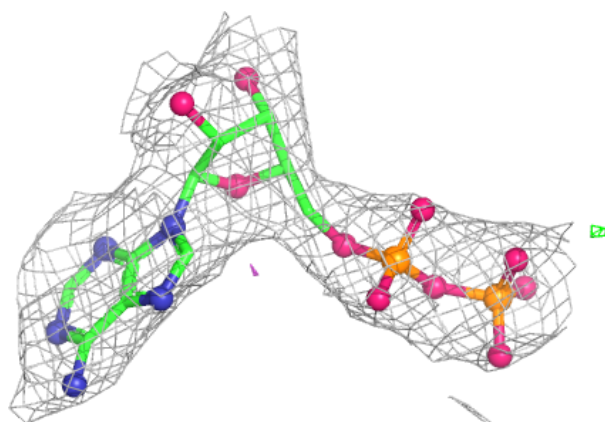
**Electron density around ADP F 1001:**

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

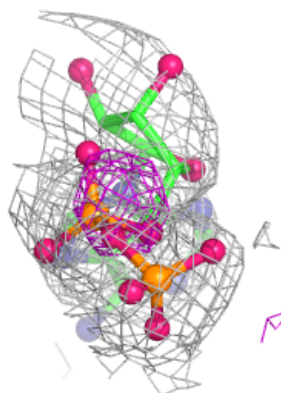
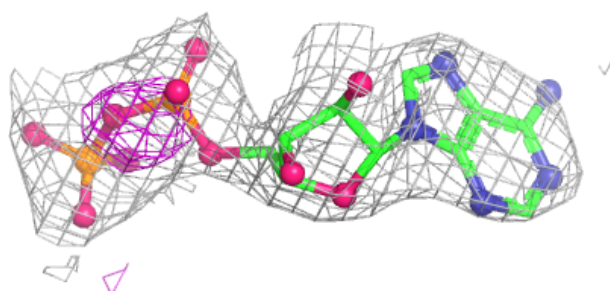
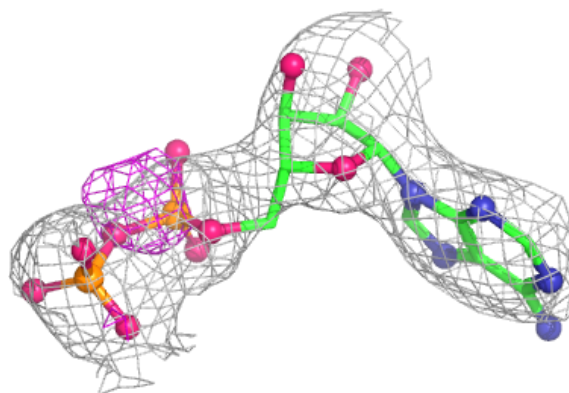


Electron density around ADP D 1001:

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

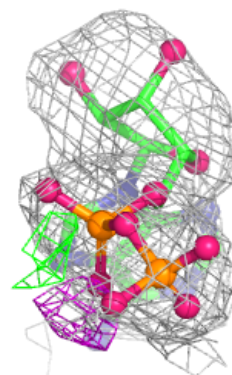
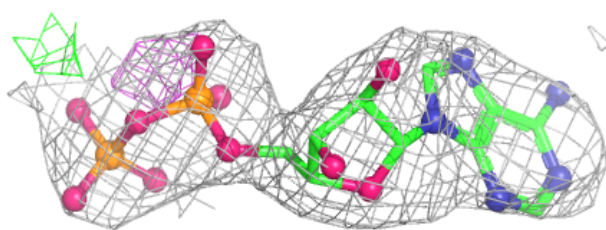
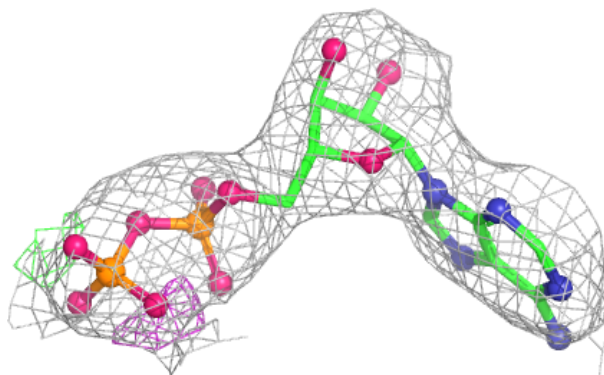
**Electron density around ADP B 1001:**

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

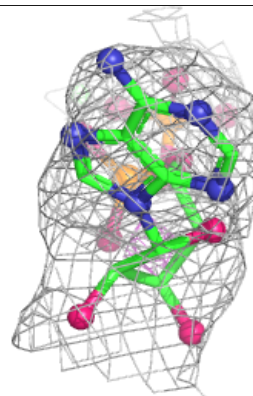
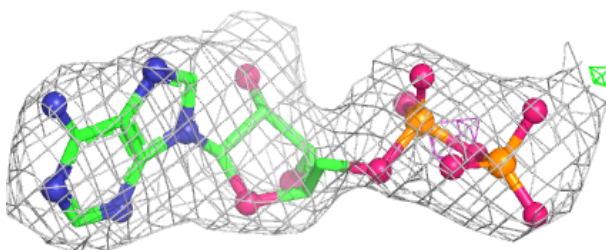
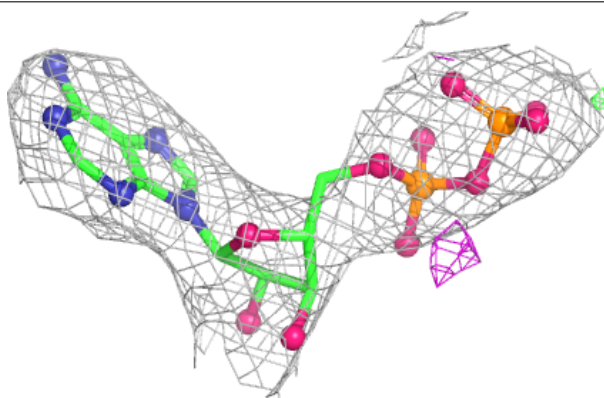


Electron density around ADP L 1001:

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

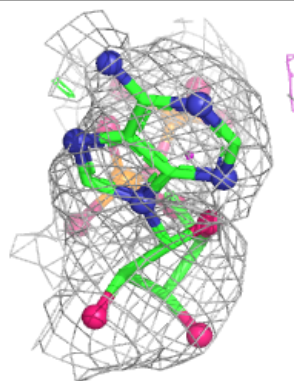
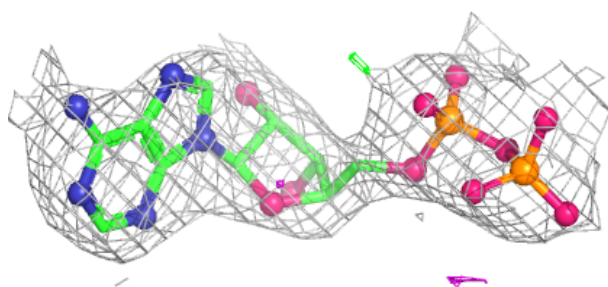
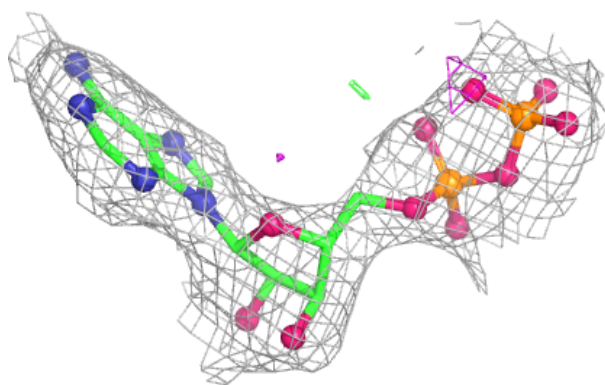
**Electron density around ADP K 1001:**

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

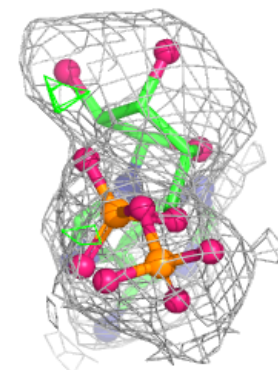
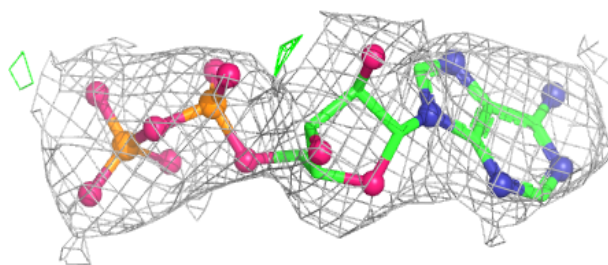
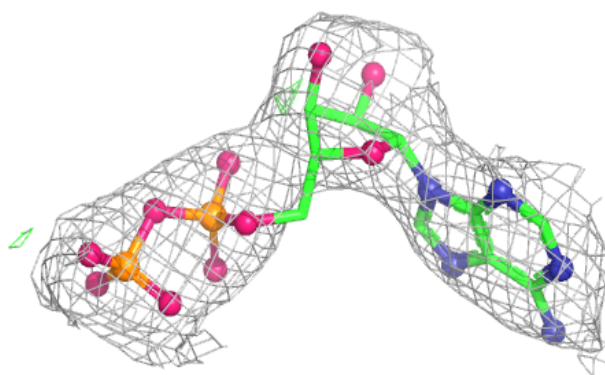


Electron density around ADP G 1001:

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

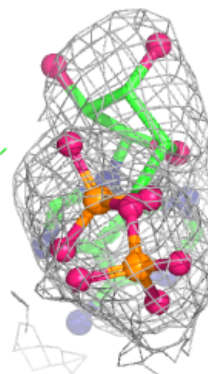
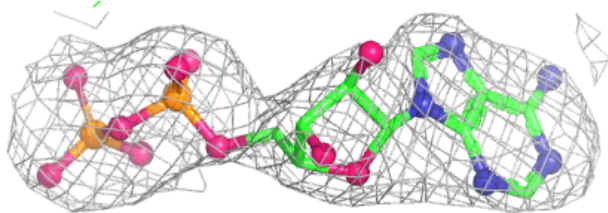
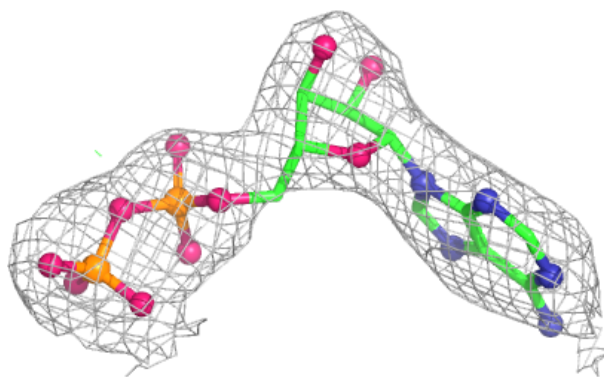
**Electron density around ADP J 1001:**

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

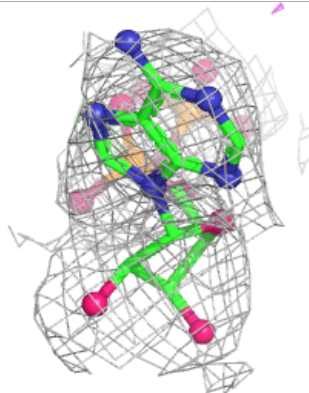
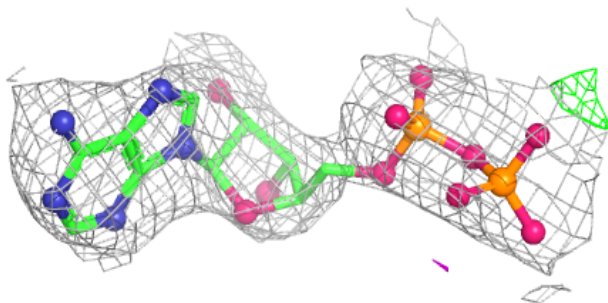
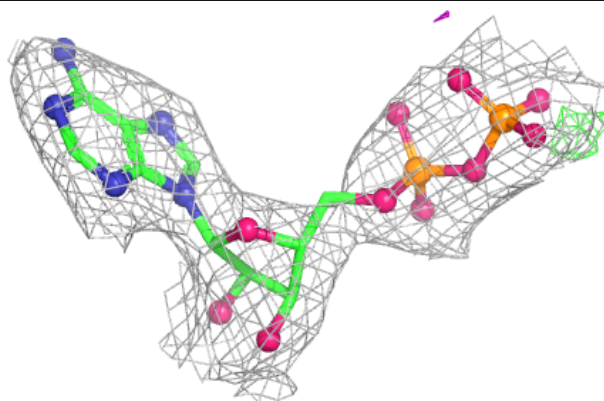


Electron density around ADP C 1001:

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

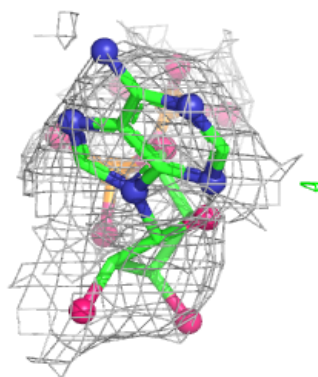
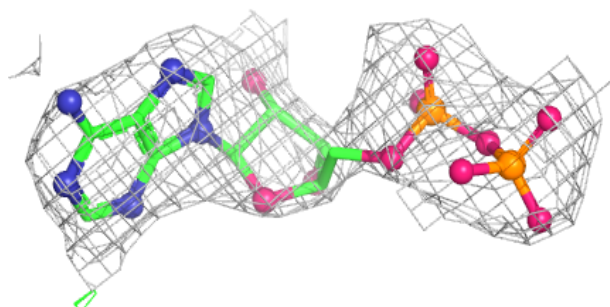
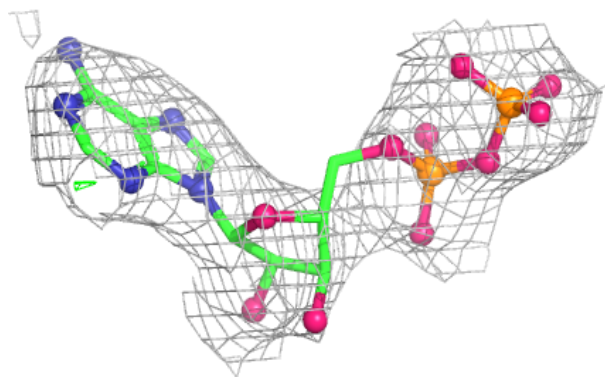
**Electron density around ADP I 1001:**

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

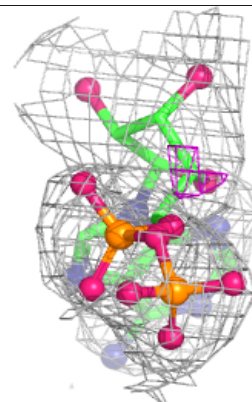
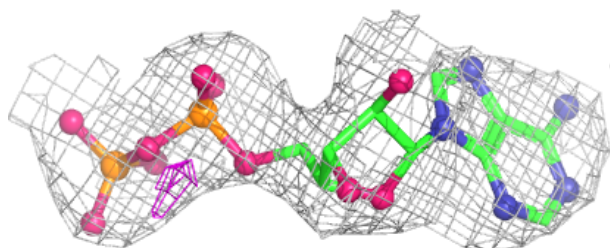
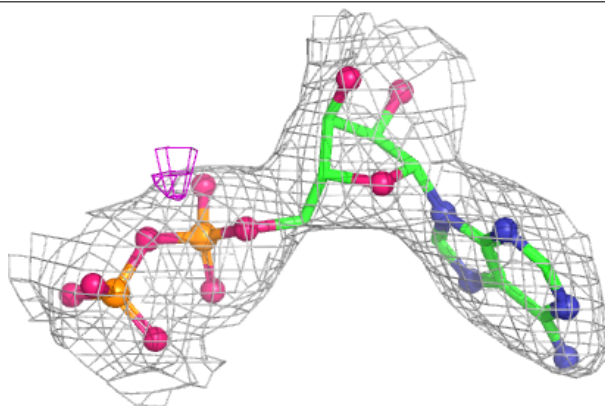


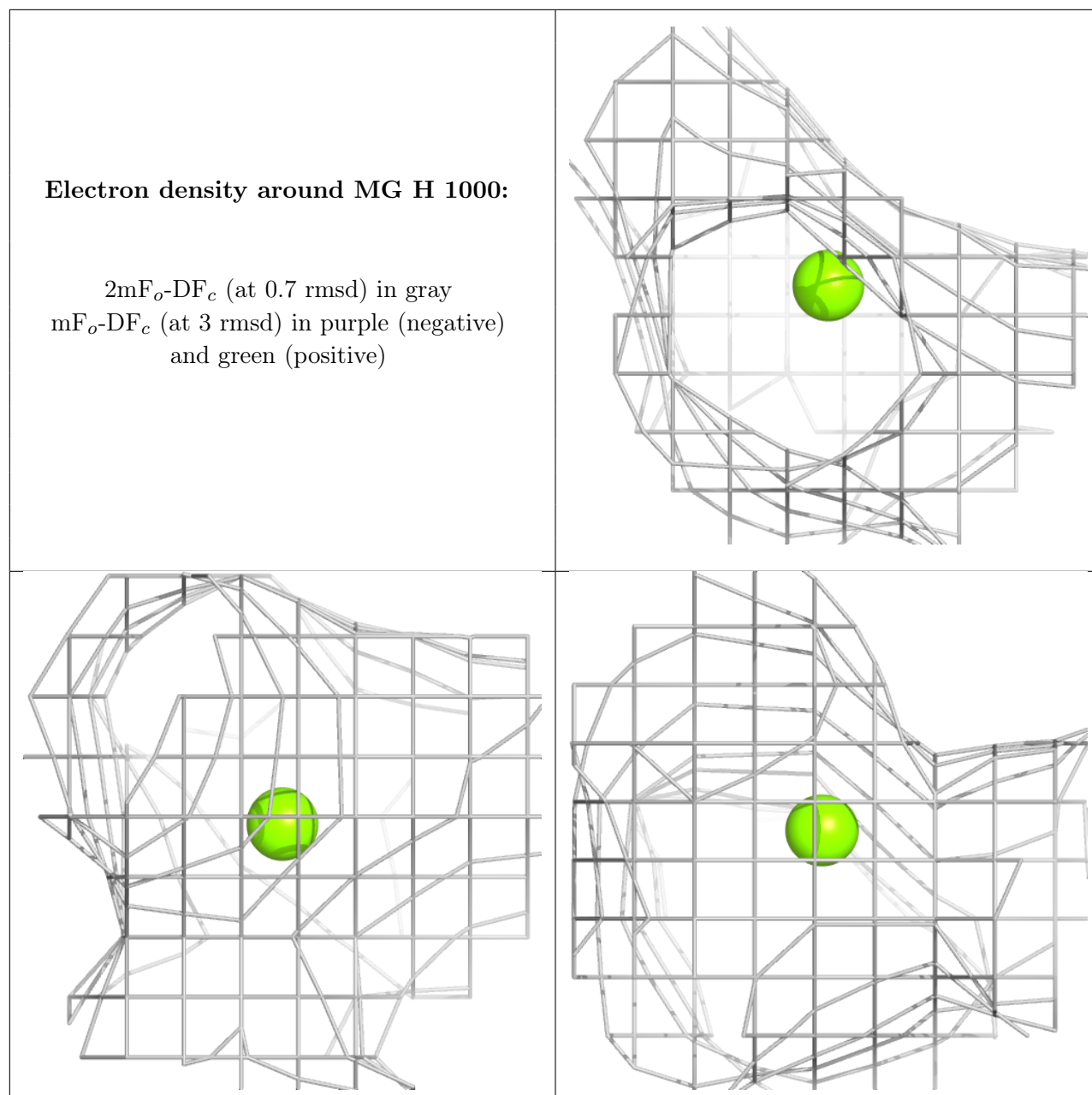
Electron density around ADP A 1001:

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

**Electron density around ADP H 1001:**

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





6.5 Other polymers ⓘ

There are no such residues in this entry.