



# Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 01:44 am BST

PDB ID : 2BUF  
Title : Arginine Feed-Back Inhibitable Acetylglutamate Kinase  
Authors : Ramon-Maiques, S.; Fernandez-Murga, M.L.; Vagin, A.; Fita, I.; Rubio, V.  
Deposited on : 2005-06-12  
Resolution : 2.95 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

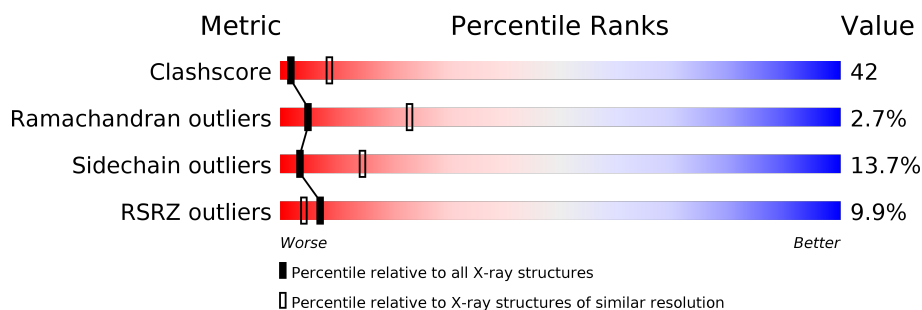
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.95 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	300	<div> <div>3%</div> <div>45% 44% 8% . .</div> </div>
1	B	300	<div> <div>3%</div> <div>46% 46% 7% . .</div> </div>
1	C	300	<div> <div>56% 37% 6%</div> </div>
1	D	300	<div> <div>60% 31% 7% .</div> </div>
1	E	300	<div> <div>5%</div> <div>48% 40% 8% .</div> </div>
1	F	300	<div> <div>7%</div> <div>47% 41% 9% .</div> </div>
1	G	300	<div> <div>8%</div> <div>48% 41% 8% . .</div> </div>

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Mol	Chain	Length	Quality of chain
1	H	300	
1	I	300	
1	J	300	
1	K	300	
1	L	300	

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
2	NLG	F	1300	-	-	-	X
2	NLG	H	1299	-	-	X	X
2	NLG	K	1298	-	-	-	X
3	ADP	H	1297	-	-	-	X
3	ADP	J	1298	-	-	X	-

## 2 Entry composition

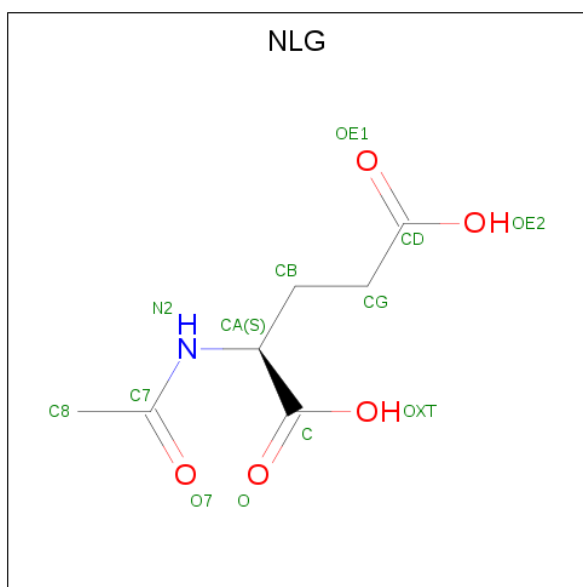
There are 5 unique types of molecules in this entry. The entry contains 25923 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ACETYLGLUTAMATE KINASE.

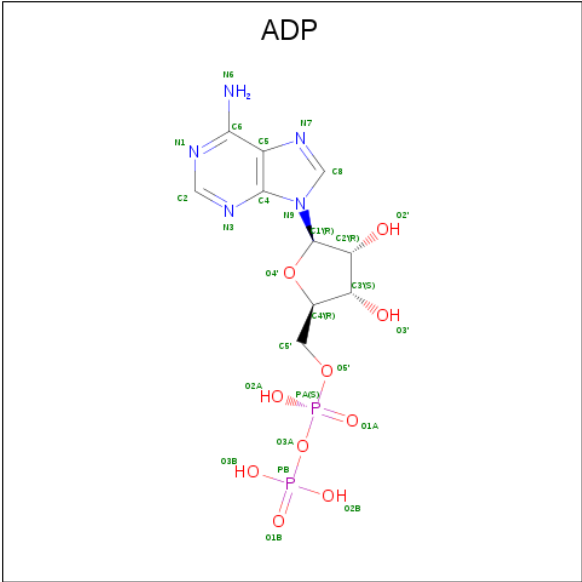
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	292	Total	C	N	O	S	0	0	0
			2159	1359	382	408	10			
1	B	297	Total	C	N	O	S	0	0	1
			2177	1371	379	416	11			
1	C	299	Total	C	N	O	S	0	0	1
			2201	1386	385	419	11			
1	D	295	Total	C	N	O	S	0	0	1
			2170	1367	381	412	10			
1	E	288	Total	C	N	O	S	0	0	1
			2106	1327	368	401	10			
1	F	292	Total	C	N	O	S	0	0	1
			2131	1343	373	405	10			
1	G	298	Total	C	N	O	S	0	0	1
			2186	1377	380	418	11			
1	H	296	Total	C	N	O	S	0	0	1
			2173	1370	377	415	11			
1	I	289	Total	C	N	O	S	0	0	1
			2110	1331	366	403	10			
1	J	280	Total	C	N	O	S	0	0	1
			2015	1266	354	385	10			
1	K	274	Total	C	N	O	S	0	0	1
			1918	1206	339	365	8			
1	L	294	Total	C	N	O	S	0	0	1
			2163	1363	380	410	10			

- Molecule 2 is N-ACETYL-L-GLUTAMATE (three-letter code: NLG) (formula: C<sub>7</sub>H<sub>11</sub>NO<sub>5</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			13	7	1	5		
2	B	1	Total	C	N	O	0	0
			13	7	1	5		
2	D	1	Total	C	N	O	0	0
			13	7	1	5		
2	E	1	Total	C	N	O	0	0
			13	7	1	5		
2	F	1	Total	C	N	O	0	0
			13	7	1	5		
2	G	1	Total	C	N	O	0	0
			13	7	1	5		
2	H	1	Total	C	N	O	0	0
			13	7	1	5		
2	I	1	Total	C	N	O	0	0
			13	7	1	5		
2	K	1	Total	C	N	O	0	0
			13	7	1	5		
2	L	1	Total	C	N	O	0	0
			13	7	1	5		

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



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

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	1	Total	Mg	0	0
			1	1		
4	D	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	1	Total 1	Mg 1	0	0
4	H	1	Total 1	Mg 1	0	0
4	B	1	Total 1	Mg 1	0	0
4	I	1	Total 1	Mg 1	0	0
4	C	1	Total 1	Mg 1	0	0
4	L	1	Total 1	Mg 1	0	0

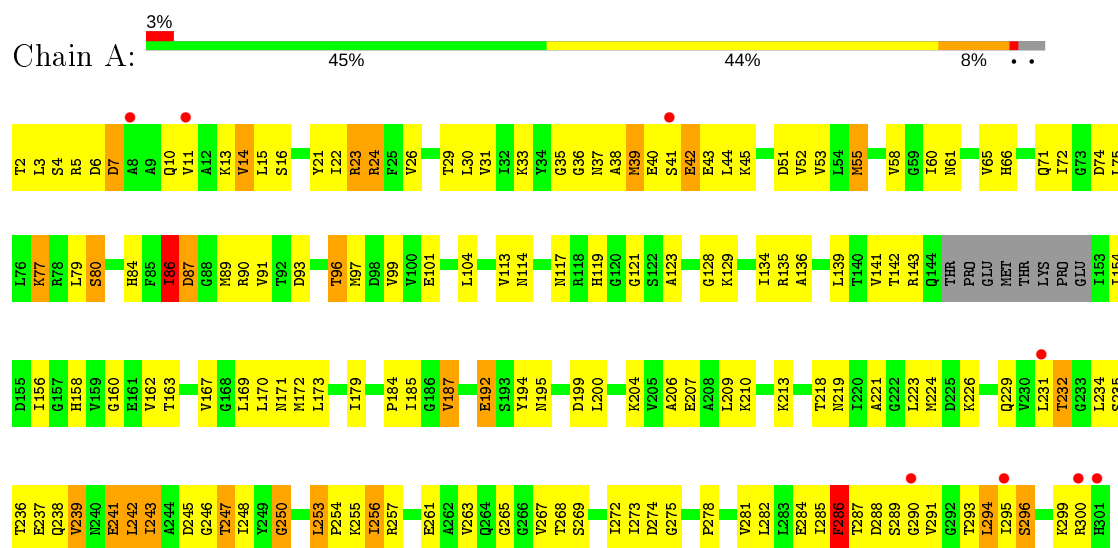
- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	G	1	Total 1	Cl 1	0	0
5	D	1	Total 1	Cl 1	0	0
5	H	1	Total 1	Cl 1	0	0
5	B	1	Total 1	Cl 1	0	0
5	C	1	Total 1	Cl 1	0	0
5	L	1	Total 1	Cl 1	0	0

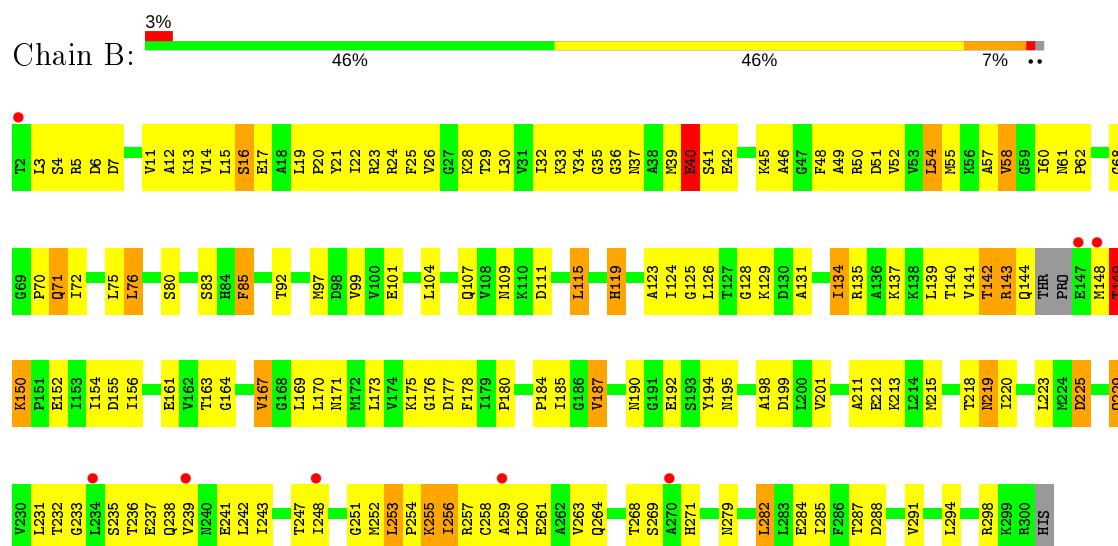
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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: ACETYLGLUTAMATE KINASE



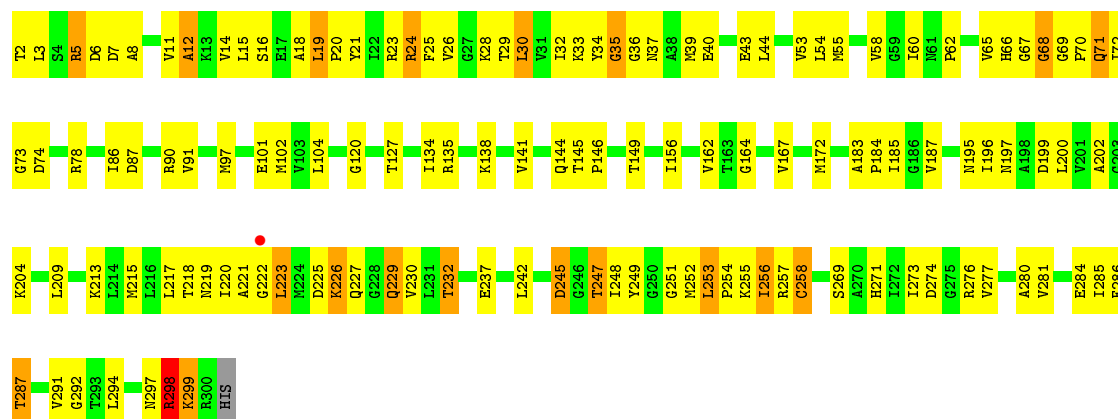
#### • Molecule 1: ACETYLGLUTAMATE KINASE



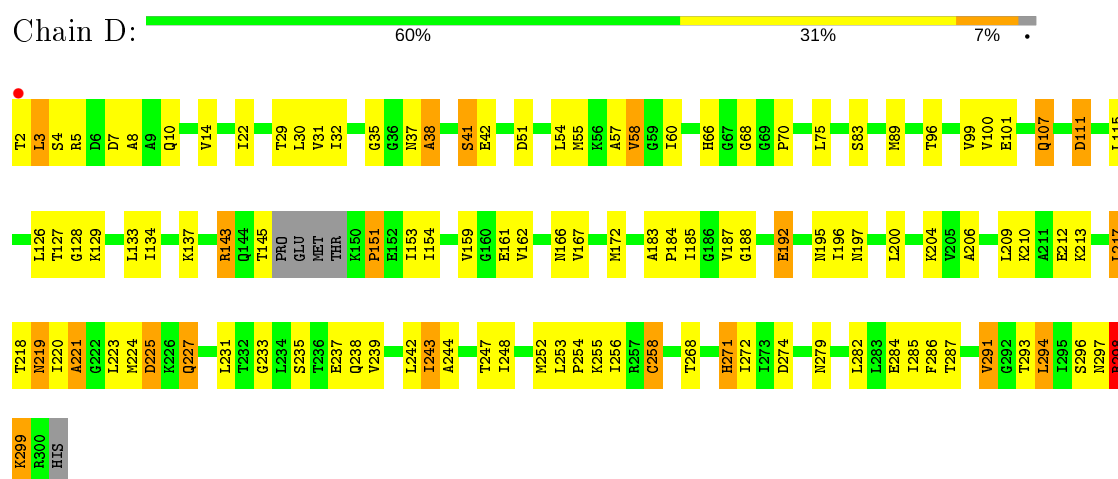
#### • Molecule 1: ACETYLGLUTAMATE KINASE



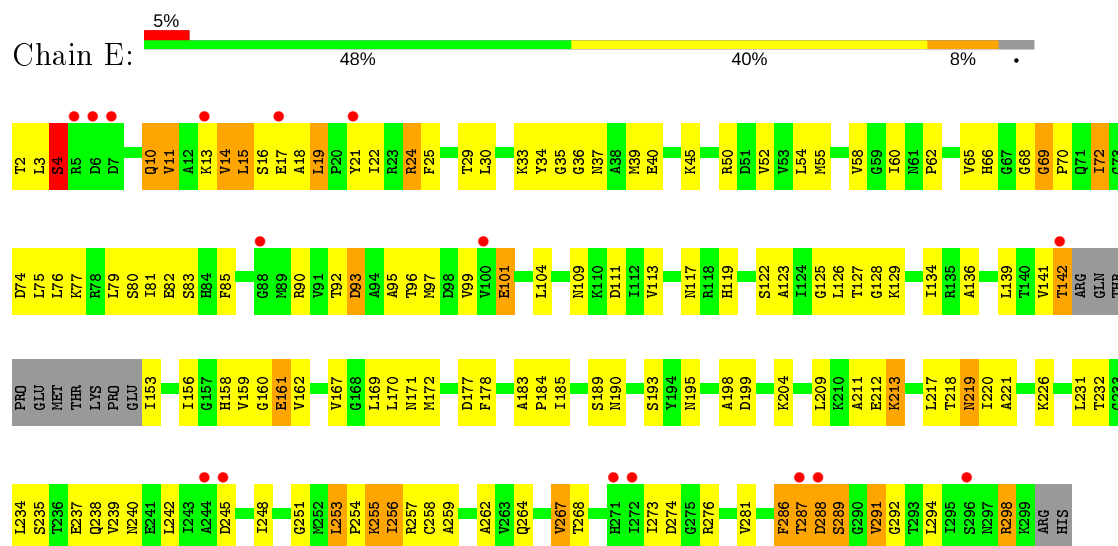




• Molecule 1: ACETYLGLUTAMATE KINASE

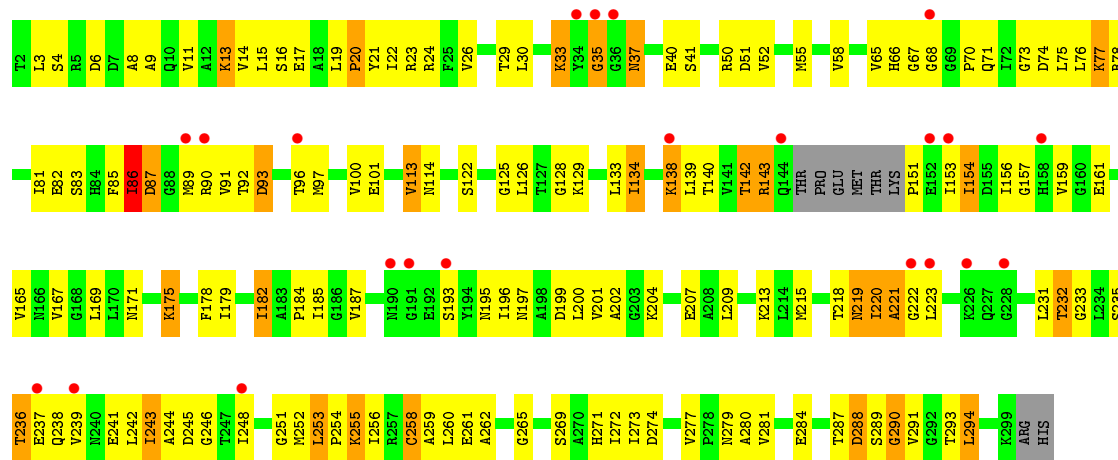


• Molecule 1: ACETYLGLUTAMATE KINASE

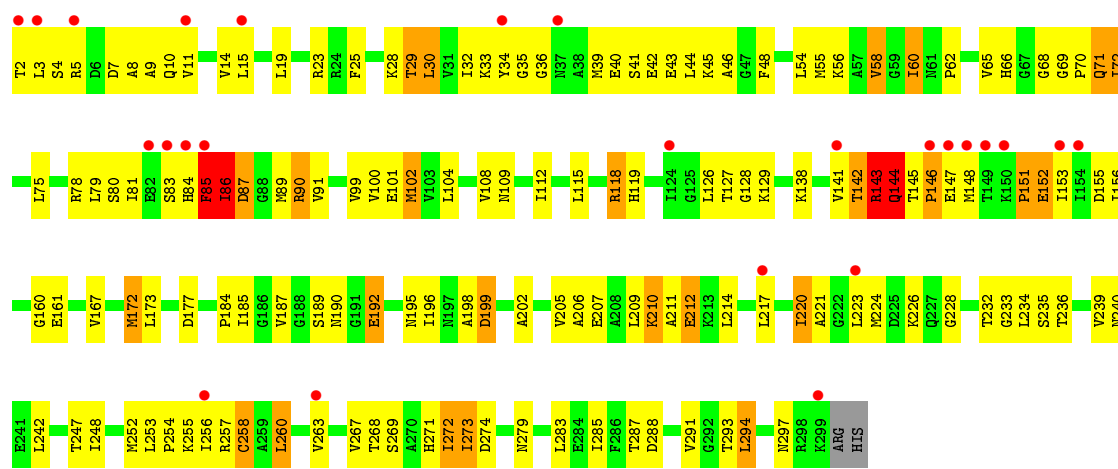


• Molecule 1: ACETYLGLUTAMATE KINASE

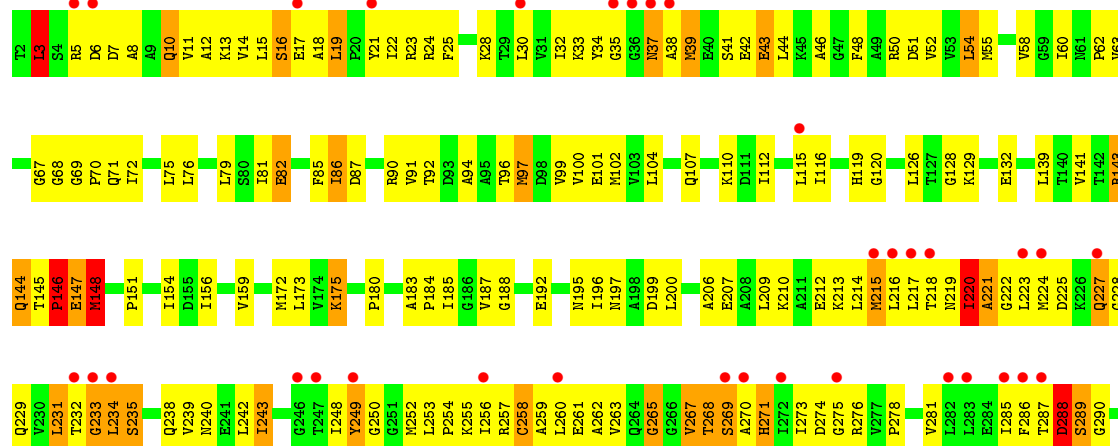


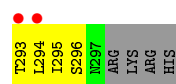


• Molecule 1: ACETYLGLUTAMATE KINASE

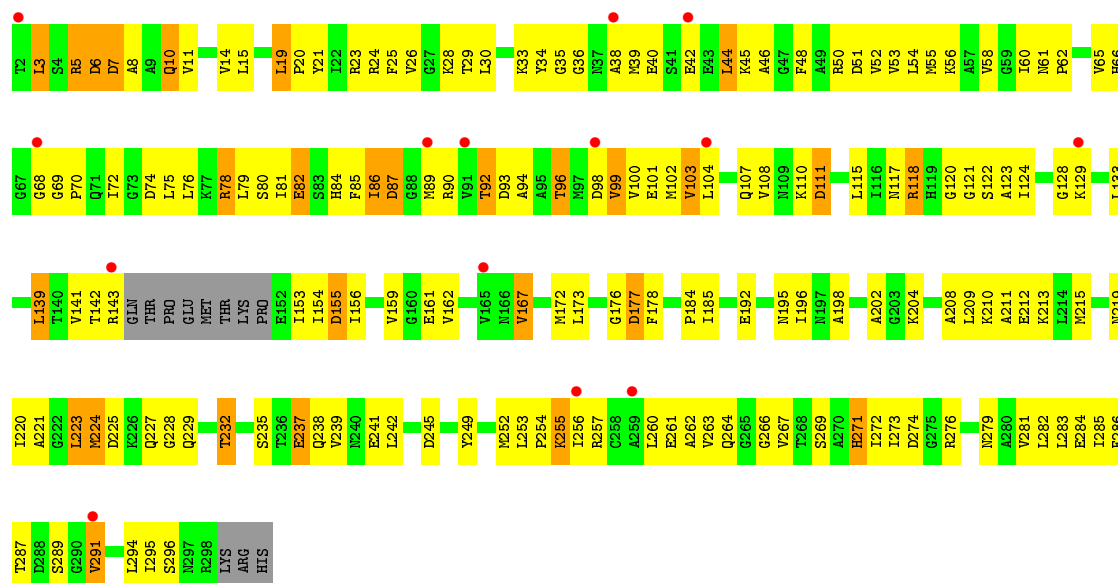


• Molecule 1: ACETYLGLUTAMATE KINASE

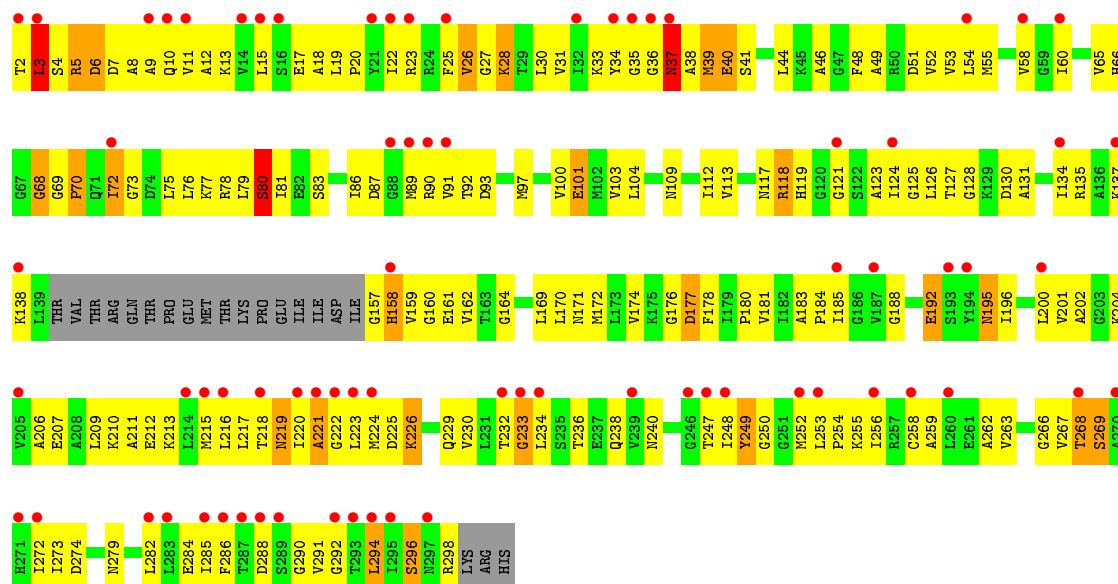




● Molecule 1: ACETYLGLUTAMATE KINASE

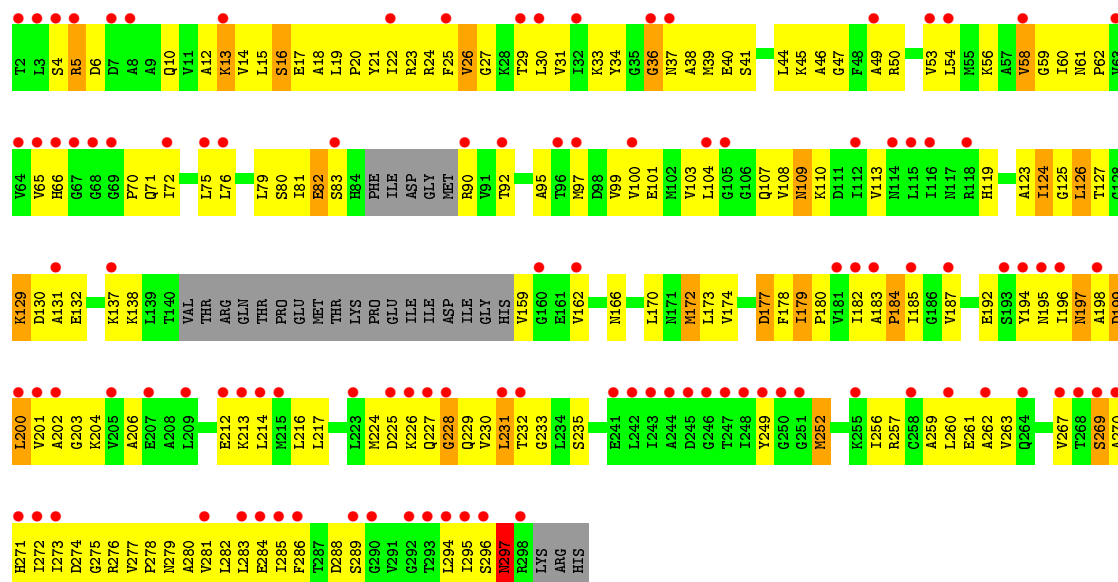


● Molecule 1: ACETYLGLUTAMATE KINASE

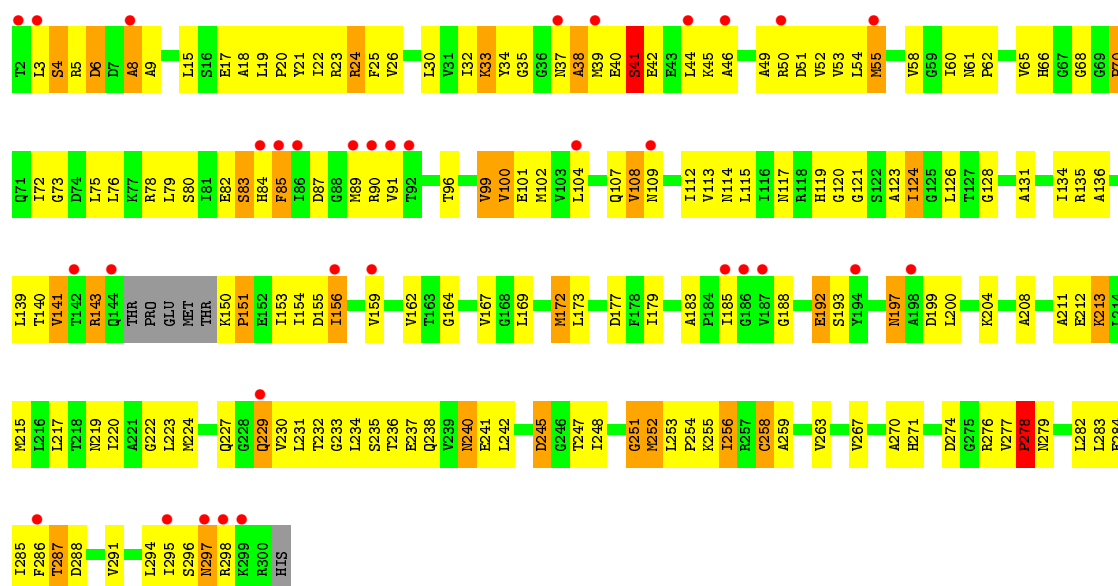
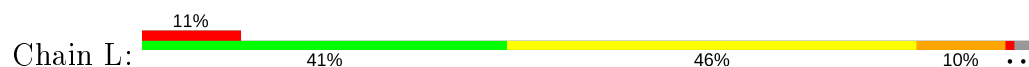


● Molecule 1: ACETYLGLUTAMATE KINASE





• Molecule 1: ACETYLGLUTAMATE KINASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	71.86 Å 98.78 Å 162.90 Å 91.49° 92.03° 107.56°	Depositor
Resolution (Å)	18.00 – 2.95 80.13 – 2.80	Depositor EDS
% Data completeness (in resolution range)	96.7 (18.00-2.95) 96.1 (80.13-2.80)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.73 (at 2.82 Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.249 , 0.267 0.240 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	78.7	Xtriage
Anisotropy	0.093	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 79.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.009 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	25923	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.45% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality

### 5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.54	0/2179	0.90	2/2940 (0.1%)
1	B	0.55	0/2197	0.94	5/2969 (0.2%)
1	C	0.57	0/2223	0.85	3/3005 (0.1%)
1	D	0.56	0/2190	0.89	3/2958 (0.1%)
1	E	0.55	1/2125 (0.0%)	0.95	5/2872 (0.2%)
1	F	0.46	0/2151	0.86	3/2907 (0.1%)
1	G	0.50	0/2208	0.91	6/2987 (0.2%)
1	H	0.54	0/2195	0.96	5/2969 (0.2%)
1	I	0.53	0/2129	0.91	4/2878 (0.1%)
1	J	0.50	0/2033	0.89	2/2747 (0.1%)
1	K	0.57	2/1934 (0.1%)	0.87	3/2620 (0.1%)
1	L	0.52	0/2183	0.88	2/2948 (0.1%)
All	All	0.53	3/25747 (0.0%)	0.90	43/34800 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	G	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	138	LYS	N-CA	10.40	1.67	1.46
1	E	4	SER	C-O	-5.61	1.12	1.23
1	K	137	LYS	CA-C	5.45	1.67	1.52

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	149	THR	N-CA-C	10.29	138.78	111.00
1	E	298	ARG	N-CA-C	9.62	136.97	111.00
1	D	298	ARG	N-CA-C	-9.19	86.20	111.00
1	E	3	LEU	N-CA-C	-7.76	90.04	111.00
1	K	4	SER	N-CA-C	7.48	131.19	111.00
1	H	148	MET	N-CA-C	7.43	131.06	111.00
1	K	233	GLY	N-CA-C	7.04	130.71	113.10
1	L	8	ALA	N-CA-C	-7.04	92.00	111.00
1	F	290	GLY	N-CA-C	-6.90	95.84	113.10
1	E	142	THR	N-CA-C	6.76	129.26	111.00
1	B	40	GLU	N-CA-C	6.47	128.47	111.00
1	G	145	THR	N-CA-C	-6.45	93.59	111.00
1	H	19	LEU	N-CA-C	6.31	128.04	111.00
1	C	35	GLY	N-CA-C	-6.25	97.48	113.10
1	A	42	GLU	N-CA-C	6.24	127.85	111.00
1	B	148	MET	N-CA-C	-6.21	94.23	111.00
1	H	288	ASP	N-CA-C	-6.08	94.58	111.00
1	H	3	LEU	CA-CB-CG	-6.08	101.32	115.30
1	H	220	ILE	N-CA-C	-6.05	94.66	111.00
1	G	87	ASP	N-CA-C	5.98	127.14	111.00
1	A	86	ILE	CB-CA-C	-5.85	99.91	111.60
1	E	3	LEU	C-N-CA	5.79	136.18	121.70
1	K	137	LYS	O-C-N	5.74	131.88	122.70
1	L	298	ARG	N-CA-C	-5.62	95.82	111.00
1	D	8	ALA	N-CA-C	-5.60	95.89	111.00
1	J	3	LEU	CA-CB-CG	-5.58	102.47	115.30
1	F	86	ILE	N-CA-C	5.53	125.94	111.00
1	G	143	ARG	N-CA-C	5.42	125.62	111.00
1	F	35	GLY	N-CA-C	5.37	126.53	113.10
1	C	68	GLY	N-CA-C	5.34	126.46	113.10
1	I	289	SER	C-N-CA	-5.27	111.23	122.30
1	B	225	ASP	N-CA-C	-5.18	97.00	111.00
1	I	291	VAL	N-CA-C	-5.18	97.02	111.00
1	I	120	GLY	N-CA-C	5.14	125.95	113.10
1	D	38	ALA	N-CA-C	5.13	124.85	111.00
1	E	69	GLY	N-CA-C	-5.11	100.34	113.10
1	B	150	LYS	N-CA-C	-5.09	97.25	111.00
1	I	96	THR	N-CA-C	-5.09	97.25	111.00
1	G	297	ASN	CA-C-N	-5.09	106.01	117.20
1	C	30	LEU	CA-CB-CG	5.08	126.99	115.30
1	G	160	GLY	N-CA-C	5.07	125.79	113.10
1	J	4	SER	N-CA-C	-5.07	97.31	111.00
1	G	35	GLY	N-CA-C	-5.02	100.54	113.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	85	PHE	Sidechain

## 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	2159	0	2259	162	0
1	B	2177	0	2265	184	0
1	C	2201	0	2302	142	0
1	D	2170	0	2272	116	0
1	E	2106	0	2196	150	0
1	F	2131	0	2213	190	0
1	G	2186	0	2278	197	0
1	H	2173	0	2270	238	0
1	I	2110	0	2195	220	0
1	J	2015	0	2071	279	0
1	K	1918	0	1917	266	0
1	L	2163	0	2265	220	0
2	A	13	0	9	0	0
2	B	13	0	9	0	0
2	D	13	0	9	1	0
2	E	13	0	9	0	0
2	F	13	0	9	3	0
2	G	13	0	9	4	0
2	H	13	0	9	6	0
2	I	13	0	9	1	0
2	K	13	0	9	4	0
2	L	13	0	9	3	0
3	B	27	0	12	2	0
3	C	27	0	12	2	0
3	D	27	0	12	0	0
3	E	27	0	12	3	0
3	F	27	0	12	2	0
3	G	27	0	12	1	0
3	H	27	0	12	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	I	27	0	12	0	0
3	J	27	0	12	13	0
3	L	27	0	12	3	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
4	I	1	0	0	0	0
4	L	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	G	1	0	0	0	0
5	H	1	0	0	0	0
5	L	1	0	0	0	0
All	All	25923	0	26713	2195	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 42.

All (2195) 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:J:282:LEU:CD2	1:K:12:ALA:HA	1.69	1.22
1:K:34:TYR:CE1	1:K:37:ASN:HB2	1.80	1.15
1:J:223:LEU:HD11	1:J:248:ILE:HG12	1.17	1.14
1:D:14:VAL:HG11	1:F:11:VAL:HG21	1.30	1.13
1:L:54:LEU:HD21	1:L:286:PHE:CZ	1.82	1.13
1:H:232:THR:HG22	1:H:233:GLY:H	1.01	1.13
1:K:5:ARG:HG3	1:K:6:ASP:H	1.03	1.12
1:L:66:HIS:CE1	1:L:183:ALA:HA	1.85	1.11
1:E:2:THR:HG23	1:E:4:SER:HB3	1.15	1.10
1:K:71:GLN:HB3	1:K:107:GLN:NE2	1.66	1.10
1:G:86:ILE:HD12	1:G:91:VAL:HG21	1.13	1.10
1:J:220:ILE:HD12	3:J:1298:ADP:H3'	1.33	1.10
1:J:223:LEU:HD11	1:J:248:ILE:CG1	1.81	1.10
1:K:124:ILE:HD12	1:K:173:LEU:HD21	1.31	1.09
1:G:86:ILE:HB	1:G:91:VAL:HG23	1.28	1.09
1:H:195:ASN:ND2	2:H:1299:NLG:H8C3	1.67	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:195:ASN:HD21	2:H:1299:NLG:H8C3	1.13	1.08
1:K:79:LEU:CD2	1:L:79:LEU:HD21	1.83	1.08
1:G:36:GLY:HA3	1:G:39:MET:CB	1.83	1.07
1:B:14:VAL:HG11	1:C:11:VAL:HG22	1.29	1.07
1:G:36:GLY:HA3	1:G:39:MET:HB3	1.36	1.07
1:D:3:LEU:HD23	1:D:3:LEU:H	1.15	1.07
1:K:260:LEU:HD23	1:K:295:ILE:HD11	1.35	1.07
1:G:223:LEU:HD13	1:G:256:ILE:HD11	1.34	1.07
1:F:218:THR:HG23	1:F:220:ILE:H	1.14	1.07
1:E:287:THR:HG22	1:E:289:SER:H	1.19	1.06
1:L:84:HIS:NE2	1:L:91:VAL:HG21	1.70	1.06
1:K:129:LYS:HD2	1:K:187:VAL:CG2	1.84	1.06
1:I:273:ILE:CD1	1:I:284:GLU:HG3	1.85	1.06
1:K:127:THR:HG22	1:K:183:ALA:HB3	1.33	1.05
1:J:220:ILE:HD12	3:J:1298:ADP:C3'	1.86	1.05
1:K:235:SER:HA	1:K:297:ASN:HD21	1.12	1.05
1:B:32:ILE:HD11	1:B:55:MET:HE1	1.33	1.05
1:J:76:LEU:HD22	1:J:81:ILE:CB	1.86	1.05
1:J:282:LEU:HD23	1:K:12:ALA:HA	1.34	1.04
1:E:2:THR:CG2	1:E:4:SER:HB3	1.87	1.03
1:G:36:GLY:CA	1:G:39:MET:HB3	1.86	1.03
1:G:118:ARG:HA	1:G:118:ARG:HH11	1.21	1.03
1:J:79:LEU:O	1:J:80:SER:HB2	1.59	1.03
1:K:37:ASN:ND2	1:K:40:GLU:HG2	1.73	1.02
1:H:141:VAL:HG21	1:H:156:ILE:HD12	1.41	1.02
1:J:285:ILE:HG22	1:J:286:PHE:CD1	1.95	1.01
1:J:15:LEU:HD13	1:K:15:LEU:HD21	1.43	1.01
1:B:13:LYS:O	1:B:17:GLU:HG3	1.61	1.00
1:J:282:LEU:HD23	1:K:12:ALA:CA	1.90	1.00
1:G:253:LEU:HB2	1:G:254:PRO:HD3	1.41	1.00
1:G:86:ILE:CD1	1:G:91:VAL:HG21	1.92	1.00
1:B:54:LEU:HD21	1:C:15:LEU:HD23	1.44	1.00
1:J:54:LEU:HD23	1:J:282:LEU:HD13	1.41	1.00
1:H:257:ARG:O	1:H:261:GLU:HG3	1.61	1.00
1:H:92:THR:HG21	1:H:97:MET:CE	1.92	1.00
1:A:22:ILE:HG23	1:A:58:VAL:HG13	1.41	0.99
1:H:96:THR:O	1:H:100:VAL:HG23	1.62	0.99
1:J:282:LEU:HD21	1:K:12:ALA:HA	1.42	0.98
1:C:221:ALA:HA	1:C:274:ASP:HB2	1.44	0.98
1:J:253:LEU:HB2	1:J:254:PRO:HD3	1.44	0.98
1:H:85:PHE:O	1:H:86:ILE:HG13	1.63	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:219:ASN:ND2	1:J:220:ILE:HG13	1.78	0.97
1:F:138:LYS:HE3	1:F:157:GLY:HA3	1.47	0.97
1:J:221:ALA:HB1	1:J:230:VAL:CG2	1.95	0.97
1:K:79:LEU:HD23	1:L:79:LEU:HD21	1.46	0.97
1:E:97:MET:HE1	1:E:195:ASN:N	1.79	0.97
1:L:54:LEU:HD21	1:L:286:PHE:CE2	2.00	0.96
1:B:14:VAL:HG11	1:C:11:VAL:CG2	1.96	0.96
1:E:35:GLY:HA2	1:E:39:MET:CG	1.95	0.96
1:E:37:ASN:HB2	1:E:219:ASN:OD1	1.63	0.96
1:H:39:MET:HE1	1:H:217:LEU:CG	1.96	0.95
1:E:35:GLY:HA2	1:E:39:MET:SD	2.07	0.95
1:G:118:ARG:HA	1:G:118:ARG:NH1	1.80	0.95
1:G:142:THR:CG2	1:G:143:ARG:N	2.26	0.95
1:K:60:ILE:O	1:K:62:PRO:HD3	1.65	0.95
1:G:86:ILE:HB	1:G:91:VAL:CG2	1.96	0.94
1:K:5:ARG:HG3	1:K:6:ASP:N	1.82	0.94
1:B:248:ILE:HG21	1:B:256:ILE:HD11	1.48	0.94
1:H:232:THR:HG22	1:H:233:GLY:N	1.83	0.94
1:H:90:ARG:HB3	2:H:1299:NLG:H8C2	1.48	0.94
1:J:221:ALA:HB1	1:J:230:VAL:HG21	1.50	0.94
1:G:142:THR:HG23	1:G:143:ARG:N	1.80	0.94
1:K:129:LYS:NZ	1:K:187:VAL:HG11	1.83	0.93
1:I:55:MET:CE	1:I:285:ILE:HD11	1.98	0.93
1:K:196:ILE:HG22	1:K:200:LEU:HD22	1.51	0.93
1:I:117:ASN:HD21	1:I:123:ALA:H	1.16	0.92
1:J:137:LYS:HG2	1:J:138:LYS:N	1.84	0.92
1:J:3:LEU:HD22	1:K:21:TYR:CE2	2.03	0.92
1:I:55:MET:HE2	1:I:285:ILE:HD11	1.48	0.92
1:K:109:ASN:HD22	1:K:109:ASN:C	1.72	0.92
1:K:196:ILE:CG2	1:K:200:LEU:HD22	2.00	0.92
1:B:34:TYR:OH	1:B:45:LYS:HA	1.68	0.92
1:K:129:LYS:HD2	1:K:187:VAL:HG21	1.50	0.92
1:E:2:THR:HG23	1:E:4:SER:CB	1.99	0.92
1:L:84:HIS:CD2	1:L:91:VAL:HG21	2.05	0.91
1:I:101:GLU:HA	1:I:185:ILE:CD1	2.01	0.91
1:A:238:GLN:O	1:A:241:GLU:HG3	1.70	0.91
1:H:238:GLN:O	1:H:242:LEU:HG	1.71	0.91
1:I:273:ILE:HD13	1:I:284:GLU:HG3	1.51	0.91
1:E:33:LYS:HE3	1:E:199:ASP:OD2	1.70	0.91
1:I:167:VAL:HG12	1:I:209:LEU:HD23	1.51	0.91
1:K:72:ILE:HD11	1:K:104:LEU:HG	1.53	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:37:ASN:HD21	1:K:40:GLU:HG2	1.28	0.91
1:H:232:THR:CG2	1:H:233:GLY:H	1.84	0.91
1:H:70:PRO:HD2	1:H:71:GLN:OE1	1.70	0.90
1:E:167:VAL:HG13	1:E:209:LEU:HD23	1.52	0.90
1:H:144:GLN:HG2	1:H:151:PRO:HG3	1.53	0.90
1:H:290:GLY:HA3	1:H:294:LEU:HD22	1.52	0.90
1:J:282:LEU:HD23	1:K:12:ALA:CB	2.01	0.90
1:J:36:GLY:H	1:J:68:GLY:HA3	1.35	0.90
1:F:133:LEU:HD21	1:F:182:ILE:HG21	1.54	0.89
1:B:36:GLY:HA3	3:B:1300:ADP:O3B	1.71	0.89
1:H:33:LYS:HB3	1:H:216:LEU:HD12	1.54	0.89
1:K:178:PHE:O	1:K:180:PRO:HD3	1.73	0.89
1:A:97:MET:HE1	1:A:195:ASN:HB2	1.53	0.89
1:H:39:MET:HE1	1:H:217:LEU:HG	1.52	0.89
1:B:35:GLY:HA2	1:B:39:MET:HE3	1.55	0.89
1:H:195:ASN:HD21	2:H:1299:NLG:C8	1.86	0.89
1:J:15:LEU:HD13	1:K:15:LEU:CD2	2.03	0.88
1:J:223:LEU:CD2	1:J:248:ILE:HD11	2.03	0.88
1:E:235:SER:H	1:E:238:GLN:HE21	1.18	0.88
1:J:232:THR:HG22	1:J:233:GLY:H	1.37	0.88
1:J:223:LEU:HD11	1:J:248:ILE:CD1	2.04	0.88
1:H:92:THR:HG21	1:H:97:MET:HE3	1.56	0.88
1:K:296:SER:O	1:K:297:ASN:HB2	1.74	0.88
1:I:273:ILE:HD11	1:I:284:GLU:HG3	1.56	0.87
1:J:285:ILE:CG2	1:J:286:PHE:CE1	2.58	0.87
1:A:117:ASN:HD21	1:A:123:ALA:H	1.19	0.87
1:B:287:THR:HG22	1:B:288:ASP:N	1.90	0.87
1:G:86:ILE:HG22	1:G:87:ASP:H	1.40	0.87
1:F:167:VAL:HG23	1:F:171:ASN:ND2	1.88	0.87
1:K:124:ILE:HD11	1:L:169:LEU:HD11	1.56	0.87
1:J:30:LEU:CD2	1:J:213:LYS:HB2	2.04	0.87
1:D:248:ILE:HD13	1:D:256:ILE:CD1	2.05	0.86
1:G:39:MET:CE	1:G:44:LEU:HD23	2.05	0.86
1:K:129:LYS:HD2	1:K:187:VAL:HG22	1.56	0.86
1:G:148:MET:CE	1:G:152:GLU:HB3	2.05	0.86
1:I:256:ILE:HG22	1:I:260:LEU:HD12	1.55	0.86
1:K:5:ARG:CG	1:K:6:ASP:H	1.86	0.86
1:K:270:ALA:HB3	1:K:295:ILE:CG2	2.06	0.86
1:J:35:GLY:O	1:J:39:MET:CE	2.23	0.85
1:K:76:LEU:HG	1:K:99:VAL:HG11	1.58	0.85
1:B:129:LYS:HD3	1:B:187:VAL:HG13	1.59	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:25:PHE:HA	1:H:28:LYS:HG2	1.56	0.85
1:J:11:VAL:HG22	1:K:14:VAL:HG13	1.58	0.85
1:F:11:VAL:O	1:F:15:LEU:HG	1.75	0.85
1:I:211:ALA:O	1:I:267:VAL:HG13	1.76	0.85
1:K:129:LYS:HZ2	1:K:187:VAL:HG11	1.39	0.85
1:G:75:LEU:HG	1:G:79:LEU:HD11	1.57	0.85
1:J:220:ILE:CD1	3:J:1298:ADP:C3'	2.54	0.85
1:K:271:HIS:ND1	1:K:284:GLU:HG2	1.91	0.85
1:B:32:ILE:HD11	1:B:55:MET:CE	2.07	0.84
1:D:253:LEU:HB3	1:D:254:PRO:HD3	1.58	0.84
1:I:223:LEU:C	1:I:223:LEU:HD12	1.97	0.84
1:G:39:MET:HE3	1:G:44:LEU:HD23	1.59	0.84
1:A:22:ILE:O	1:A:26:VAL:HG23	1.76	0.84
1:H:144:GLN:CG	1:H:151:PRO:HG3	2.07	0.84
1:J:2:THR:HG22	1:J:3:LEU:H	1.42	0.84
1:K:235:SER:HA	1:K:297:ASN:ND2	1.92	0.84
1:J:285:ILE:CG2	1:J:286:PHE:CD1	2.60	0.84
1:H:21:TYR:O	1:H:24:ARG:HG2	1.77	0.84
1:H:23:ARG:HH11	1:H:23:ARG:HG3	1.42	0.84
1:E:287:THR:HG22	1:E:289:SER:N	1.93	0.83
1:E:232:THR:HG23	1:E:294:LEU:H	1.41	0.83
1:B:287:THR:HG22	1:B:288:ASP:H	1.42	0.83
1:J:118:ARG:HB3	1:J:118:ARG:HH11	1.42	0.83
1:I:117:ASN:HD21	1:I:123:ALA:N	1.76	0.83
1:J:219:ASN:HD22	1:J:220:ILE:HG13	1.41	0.83
1:E:167:VAL:HG13	1:E:209:LEU:CD2	2.08	0.83
1:K:79:LEU:HD23	1:L:79:LEU:CD2	2.08	0.83
1:B:232:THR:HG23	1:B:294:LEU:H	1.43	0.83
1:L:229:GLN:NE2	1:L:229:GLN:HA	1.93	0.83
1:A:11:VAL:HG23	1:E:14:VAL:CG1	2.07	0.83
1:H:92:THR:CG2	1:H:97:MET:HE2	2.09	0.83
1:H:39:MET:HE1	1:H:217:LEU:CD2	2.09	0.83
1:I:96:THR:O	1:I:100:VAL:HG23	1.77	0.83
1:G:211:ALA:O	1:G:267:VAL:HG13	1.79	0.82
1:I:117:ASN:ND2	1:I:123:ALA:H	1.78	0.82
1:L:85:PHE:HD2	1:L:89:MET:O	1.62	0.82
1:L:143:ARG:HD2	1:L:143:ARG:H	1.43	0.82
1:G:118:ARG:CA	1:G:118:ARG:HH11	1.92	0.82
1:J:219:ASN:HD22	1:J:219:ASN:C	1.77	0.82
1:J:248:ILE:HD13	1:J:256:ILE:HD12	1.62	0.82
1:F:271:HIS:HB3	1:F:273:ILE:HD11	1.62	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:230:VAL:HG11	1:C:292:GLY:HA2	1.60	0.81
1:J:12:ALA:HB1	1:K:282:LEU:CD1	2.10	0.81
1:J:223:LEU:HD21	1:J:248:ILE:HD11	1.60	0.81
1:J:30:LEU:HD12	1:J:60:ILE:CG2	2.10	0.81
1:L:117:ASN:HA	1:L:121:GLY:O	1.80	0.81
1:H:35:GLY:HA3	1:H:67:GLY:H	1.45	0.81
1:H:39:MET:HE3	1:H:275:GLY:HA3	1.61	0.81
1:I:101:GLU:HA	1:I:185:ILE:HD11	1.63	0.81
1:K:271:HIS:ND1	1:K:284:GLU:CG	2.44	0.81
1:K:273:ILE:HG22	1:K:274:ASP:N	1.96	0.81
1:F:236:THR:HG22	1:F:237:GLU:N	1.96	0.81
1:L:68:GLY:O	1:L:70:PRO:HD2	1.81	0.81
1:C:2:THR:HG22	1:C:3:LEU:H	1.44	0.80
1:H:97:MET:HE2	1:H:97:MET:HA	1.62	0.80
1:C:28:LYS:CG	1:C:29:THR:H	1.94	0.80
1:K:260:LEU:HD23	1:K:295:ILE:CD1	2.11	0.80
1:G:129:LYS:HG2	1:G:187:VAL:CG2	2.09	0.80
1:L:156:ILE:HG22	1:L:159:VAL:HG21	1.62	0.80
1:K:71:GLN:HB3	1:K:107:GLN:HE21	1.41	0.80
1:H:12:ALA:HB3	1:L:50:ARG:NH2	1.96	0.80
1:B:54:LEU:CD2	1:C:15:LEU:HD23	2.11	0.80
1:F:238:GLN:O	1:F:241:GLU:HB2	1.81	0.80
1:J:15:LEU:CD1	1:K:15:LEU:HD11	2.11	0.80
1:J:118:ARG:CB	1:J:118:ARG:HH11	1.95	0.80
1:K:273:ILE:HG22	1:K:274:ASP:H	1.46	0.80
1:D:282:LEU:O	1:D:286:PHE:HB2	1.82	0.80
1:J:285:ILE:HG22	1:J:286:PHE:CE1	2.16	0.80
1:K:37:ASN:ND2	1:K:45:LYS:HD2	1.97	0.80
1:L:141:VAL:HG21	1:L:156:ILE:HB	1.64	0.80
1:E:167:VAL:HG12	1:E:171:ASN:ND2	1.95	0.79
1:G:142:THR:O	1:G:143:ARG:HB2	1.81	0.79
1:J:252:MET:CE	1:J:255:LYS:HD2	2.12	0.79
1:G:40:GLU:HG2	1:G:45:LYS:HE3	1.64	0.79
1:I:81:ILE:HG21	1:I:96:THR:HG22	1.64	0.79
1:I:223:LEU:HD23	1:I:256:ILE:HD11	1.64	0.79
1:A:39:MET:SD	1:A:275:GLY:HA3	2.21	0.79
1:D:14:VAL:HG11	1:F:11:VAL:CG2	2.10	0.79
1:J:223:LEU:HD13	1:J:256:ILE:HD11	1.65	0.79
1:K:103:VAL:HG13	1:K:107:GLN:CD	2.01	0.79
1:G:172:MET:HE3	1:H:172:MET:HG2	1.63	0.79
1:J:178:PHE:O	1:J:180:PRO:HD3	1.83	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:34:TYR:HE1	1:K:37:ASN:HB2	1.45	0.79
1:L:140:THR:HG22	1:L:153:ILE:HD13	1.64	0.79
1:L:54:LEU:CD2	1:L:282:LEU:HD21	2.12	0.79
1:C:221:ALA:CA	1:C:274:ASP:HB2	2.11	0.79
1:D:299:LYS:HG2	1:D:299:LYS:O	1.83	0.79
1:D:3:LEU:HD23	1:D:3:LEU:N	1.98	0.79
1:C:28:LYS:HG3	1:C:29:THR:H	1.47	0.79
1:K:232:THR:HG23	1:K:294:LEU:HB3	1.65	0.79
1:G:36:GLY:HA3	1:G:39:MET:HB2	1.65	0.79
1:H:22:ILE:HD11	1:H:286:PHE:CE2	2.18	0.79
1:H:69:GLY:N	1:H:70:PRO:HD3	1.98	0.78
1:H:197:ASN:HB3	1:H:200:LEU:HD12	1.64	0.78
1:I:7:ASP:O	1:I:11:VAL:HG23	1.83	0.78
1:I:124:ILE:HD12	1:I:173:LEU:HD22	1.66	0.78
1:K:212:GLU:HG3	1:K:213:LYS:HG3	1.66	0.78
1:J:176:GLY:O	1:J:177:ASP:HB2	1.84	0.78
1:C:24:ARG:HD3	1:C:25:PHE:CZ	2.19	0.78
1:J:19:LEU:HA	1:J:22:ILE:HD12	1.65	0.78
1:B:97:MET:HE1	1:B:195:ASN:N	1.99	0.78
1:J:223:LEU:CD1	1:J:248:ILE:CD1	2.61	0.78
1:L:72:ILE:O	1:L:76:LEU:HG	1.84	0.78
1:G:86:ILE:HD12	1:G:91:VAL:CG2	2.07	0.78
1:H:234:LEU:HD23	1:H:238:GLN:HB3	1.66	0.78
1:K:197:ASN:O	1:K:201:VAL:HG23	1.84	0.78
1:L:271:HIS:HD2	1:L:284:GLU:HG2	1.48	0.78
1:A:11:VAL:HG23	1:E:14:VAL:HG12	1.66	0.77
1:G:66:HIS:O	1:G:184:PRO:HD3	1.85	0.77
1:K:174:VAL:O	1:K:177:ASP:N	2.14	0.77
1:I:21:TYR:O	1:I:24:ARG:HG2	1.84	0.77
1:A:234:LEU:CD2	1:A:239:VAL:HG23	2.15	0.77
1:A:23:ARG:HH11	1:A:23:ARG:HG2	1.48	0.77
1:G:5:ARG:NH1	1:I:291:VAL:HG22	1.99	0.77
1:D:243:ILE:HD13	1:D:244:ALA:N	2.00	0.77
1:I:79:LEU:HD13	1:J:78:ARG:HG2	1.66	0.77
1:K:72:ILE:HG12	1:K:103:VAL:HB	1.65	0.77
1:A:75:LEU:HD23	1:A:99:VAL:HG13	1.67	0.77
1:E:162:VAL:HB	1:E:204:LYS:HG3	1.66	0.77
1:F:91:VAL:HG22	1:F:156:ILE:HG12	1.67	0.77
1:E:262:ALA:O	1:E:267:VAL:HG23	1.84	0.77
1:D:242:LEU:HD22	1:D:247:THR:HG21	1.64	0.77
1:G:15:LEU:HB3	1:I:54:LEU:HD21	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:71:GLN:HG3	1:G:108:VAL:CG2	2.16	0.76
1:I:256:ILE:HD12	1:I:295:ILE:HD11	1.67	0.76
1:J:54:LEU:O	1:J:58:VAL:HG23	1.85	0.76
1:K:79:LEU:HD21	1:L:79:LEU:HD21	1.66	0.76
1:A:33:LYS:HE3	1:A:199:ASP:OD2	1.85	0.76
1:K:34:TYR:CE1	1:K:45:LYS:HE3	2.20	0.76
1:G:129:LYS:HG2	1:G:187:VAL:HG21	1.67	0.76
1:J:248:ILE:O	1:J:253:LEU:HD21	1.86	0.76
1:L:270:ALA:O	1:L:294:LEU:HD12	1.86	0.76
1:J:118:ARG:CG	1:J:118:ARG:HH11	1.98	0.76
1:D:252:MET:HE3	1:D:255:LYS:HB3	1.68	0.76
1:I:99:VAL:O	1:I:102:MET:HG2	1.86	0.76
1:B:128:GLY:HA3	1:B:185:ILE:O	1.86	0.75
1:D:30:LEU:HD22	1:D:213:LYS:HB2	1.68	0.75
1:E:10:GLN:HG2	1:E:11:VAL:N	2.01	0.75
1:E:97:MET:HE1	1:E:195:ASN:H	1.50	0.75
1:L:223:LEU:HD13	1:L:256:ILE:HD13	1.68	0.75
1:E:101:GLU:HG2	1:E:185:ILE:HD13	1.67	0.75
1:H:60:ILE:O	1:H:62:PRO:HD3	1.87	0.75
1:K:76:LEU:CG	1:K:99:VAL:HG11	2.17	0.75
1:L:19:LEU:HB3	1:L:20:PRO:HD3	1.67	0.75
1:J:37:ASN:O	1:J:40:GLU:HG3	1.85	0.75
1:C:34:TYR:O	1:C:66:HIS:HA	1.87	0.75
1:F:271:HIS:ND1	1:F:284:GLU:HG3	2.01	0.75
1:H:285:ILE:HG12	1:H:285:ILE:O	1.85	0.75
1:L:229:GLN:HE21	1:L:229:GLN:HA	1.50	0.75
1:F:89:MET:SD	1:F:139:LEU:HD21	2.26	0.74
1:J:253:LEU:HB2	1:J:254:PRO:CD	2.17	0.74
1:B:21:TYR:O	1:B:24:ARG:HG2	1.86	0.74
1:G:72:ILE:HD12	1:G:90:ARG:HH21	1.52	0.74
1:H:92:THR:CG2	1:H:97:MET:CE	2.66	0.74
1:A:22:ILE:HG23	1:A:58:VAL:CG1	2.14	0.74
1:B:12:ALA:O	1:B:16:SER:HB3	1.87	0.74
1:I:79:LEU:HD22	1:J:78:ARG:HD3	1.67	0.74
1:K:270:ALA:HB3	1:K:295:ILE:HG22	1.69	0.74
1:J:12:ALA:HB1	1:K:282:LEU:HD13	1.67	0.74
1:H:235:SER:O	1:H:239:VAL:HG23	1.87	0.74
1:H:243:ILE:HD12	1:H:257:ARG:NH2	2.03	0.74
1:J:221:ALA:CB	1:J:230:VAL:CG2	2.66	0.74
1:L:54:LEU:CD2	1:L:286:PHE:CZ	2.67	0.74
1:F:218:THR:HG23	1:F:220:ILE:N	1.99	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:12:ALA:HB3	1:L:50:ARG:HH21	1.53	0.74
1:I:11:VAL:O	1:I:15:LEU:HG	1.87	0.74
1:I:72:ILE:CG2	1:I:76:LEU:HD12	2.18	0.74
1:L:82:GLU:CG	1:L:83:SER:N	2.51	0.74
1:F:129:LYS:HA	1:F:187:VAL:HG21	1.68	0.73
1:G:84:HIS:HA	1:G:85:PHE:CE1	2.23	0.73
1:J:124:ILE:CG2	1:J:126:LEU:HD21	2.17	0.73
1:H:223:LEU:HD11	1:H:248:ILE:HG12	1.70	0.73
1:I:213:LYS:HG3	1:I:269:SER:OG	1.87	0.73
1:J:259:ALA:O	1:J:263:VAL:HG23	1.88	0.73
1:K:103:VAL:O	1:K:107:GLN:HG2	1.88	0.73
1:G:75:LEU:HG	1:G:79:LEU:CD1	2.17	0.73
1:H:34:TYR:CD2	1:H:35:GLY:N	2.56	0.73
1:J:170:LEU:O	1:J:174:VAL:HG23	1.87	0.73
1:B:11:VAL:O	1:B:14:VAL:HG12	1.88	0.73
1:B:101:GLU:HA	1:B:185:ILE:CD1	2.19	0.73
1:H:253:LEU:HB3	1:H:254:PRO:HD3	1.70	0.73
1:I:78:ARG:HG2	1:J:79:LEU:HD11	1.71	0.73
1:I:79:LEU:HD22	1:J:78:ARG:CD	2.17	0.73
1:L:231:LEU:HB3	1:L:234:LEU:HD21	1.70	0.73
1:A:218:THR:HG22	1:A:255:LYS:HE3	1.69	0.73
1:G:226:LYS:C	1:G:228:GLY:H	1.92	0.73
1:D:101:GLU:HA	1:D:185:ILE:HD11	1.71	0.73
1:D:220:ILE:O	1:D:221:ALA:HB2	1.88	0.73
1:F:76:LEU:HB3	1:F:81:ILE:O	1.89	0.73
1:K:36:GLY:O	1:K:44:LEU:HD23	1.88	0.73
1:L:232:THR:HG23	1:L:294:LEU:H	1.52	0.73
1:B:34:TYR:CE1	1:B:48:PHE:CG	2.77	0.73
1:J:232:THR:HG22	1:J:233:GLY:N	2.03	0.73
1:A:231:LEU:HD21	1:A:242:LEU:HD21	1.70	0.72
1:F:101:GLU:HA	1:F:185:ILE:HD11	1.71	0.72
1:I:117:ASN:HA	1:I:121:GLY:O	1.89	0.72
1:J:19:LEU:HD22	1:K:54:LEU:CD1	2.18	0.72
1:D:3:LEU:H	1:D:3:LEU:CD2	1.94	0.72
1:G:79:LEU:O	1:G:80:SER:HB2	1.87	0.72
1:H:92:THR:HG21	1:H:97:MET:HE2	1.68	0.72
1:C:172:MET:HG2	1:D:172:MET:HE2	1.70	0.72
1:H:143:ARG:HD3	1:H:154:ILE:HD11	1.72	0.72
1:B:34:TYR:CD1	1:B:48:PHE:CD1	2.77	0.72
1:F:196:ILE:HG22	1:F:197:ASN:N	2.04	0.72
1:L:82:GLU:CG	1:L:83:SER:H	2.01	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:240:ASN:HA	1:H:243:ILE:HG13	1.70	0.72
1:K:25:PHE:CE1	1:K:285:ILE:HA	2.24	0.72
1:A:84:HIS:CE1	1:A:91:VAL:HG21	2.23	0.72
1:D:248:ILE:HG21	1:D:256:ILE:CD1	2.20	0.72
1:D:54:LEU:HD11	1:F:15:LEU:HD12	1.72	0.72
1:F:167:VAL:HG23	1:F:171:ASN:HD21	1.53	0.72
1:H:39:MET:HE1	1:H:217:LEU:HD23	1.70	0.72
1:K:282:LEU:O	1:K:285:ILE:HG12	1.90	0.72
1:E:128:GLY:HA2	1:E:134:ILE:HD12	1.71	0.72
1:I:279:ASN:O	1:I:283:LEU:HG	1.89	0.72
1:F:3:LEU:HD11	1:F:11:VAL:HB	1.71	0.72
1:A:36:GLY:C	1:A:38:ALA:H	1.93	0.72
1:J:137:LYS:HG2	1:J:138:LYS:H	1.52	0.72
1:G:19:LEU:HD21	1:I:53:VAL:CG1	2.20	0.71
1:L:162:VAL:HB	1:L:204:LYS:HG3	1.71	0.71
1:J:282:LEU:CD2	1:K:12:ALA:CA	2.53	0.71
1:F:92:THR:HG23	1:F:96:THR:OG1	1.91	0.71
1:J:41:SER:HB3	1:J:44:LEU:HG	1.73	0.71
1:B:149:THR:HG22	1:B:150:LYS:N	2.06	0.71
1:B:218:THR:HG23	1:B:220:ILE:H	1.56	0.71
1:G:223:LEU:CD1	1:G:256:ILE:HD11	2.19	0.71
1:G:143:ARG:CZ	1:G:151:PRO:HG3	2.20	0.71
1:H:100:VAL:HG12	1:H:104:LEU:HD12	1.73	0.71
1:K:273:ILE:HD11	1:K:284:GLU:CD	2.11	0.71
1:A:143:ARG:HB2	1:A:154:ILE:HD13	1.72	0.70
1:B:5:ARG:HG3	1:C:291:VAL:HG11	1.73	0.70
1:E:55:MET:O	1:E:60:ILE:HB	1.91	0.70
1:F:30:LEU:HD22	1:F:213:LYS:HB2	1.72	0.70
1:L:253:LEU:HB2	1:L:254:PRO:HD3	1.73	0.70
1:I:55:MET:HE3	1:I:281:VAL:HG12	1.73	0.70
1:K:172:MET:SD	1:L:172:MET:HG3	2.32	0.70
1:A:234:LEU:HD23	1:A:239:VAL:HG23	1.73	0.70
1:G:272:ILE:HG23	1:G:293:THR:HB	1.72	0.70
1:J:125:GLY:O	1:J:126:LEU:HD23	1.90	0.70
1:K:109:ASN:HD21	1:K:125:GLY:HA3	1.55	0.70
1:J:118:ARG:HB3	1:J:118:ARG:NH1	2.07	0.70
1:D:219:ASN:HD22	1:D:219:ASN:C	1.93	0.70
1:A:86:ILE:HD12	1:A:156:ILE:HD11	1.73	0.70
1:B:34:TYR:CD2	1:B:39:MET:HE3	2.26	0.70
1:C:23:ARG:HA	1:C:26:VAL:HG23	1.74	0.70
1:G:8:ALA:HB2	1:I:287:THR:HG21	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:279:ASN:O	1:L:283:LEU:HG	1.92	0.70
1:L:82:GLU:HG2	1:L:83:SER:H	1.55	0.70
1:G:36:GLY:C	1:G:39:MET:HB3	2.12	0.70
1:B:35:GLY:HA2	1:B:39:MET:CE	2.22	0.70
1:B:3:LEU:HB2	1:C:287:THR:HG23	1.72	0.70
1:F:85:PHE:HB2	1:F:90:ARG:HA	1.74	0.70
1:J:225:ASP:OD2	1:J:229:GLN:HB2	1.91	0.70
1:J:15:LEU:HD13	1:K:15:LEU:HD11	1.74	0.69
1:K:124:ILE:HG22	1:K:126:LEU:HD11	1.72	0.69
1:A:93:ASP:OD2	1:A:96:THR:HG23	1.92	0.69
1:B:124:ILE:HG22	1:B:126:LEU:HG	1.73	0.69
1:G:65:VAL:HG21	1:G:202:ALA:HA	1.75	0.69
1:H:220:ILE:HG13	1:H:224:MET:HE2	1.75	0.69
1:L:68:GLY:H	2:L:1302:NLG:HGC2	1.57	0.69
1:K:197:ASN:HA	2:K:1298:NLG:OE1	1.92	0.69
1:G:85:PHE:CD1	1:G:85:PHE:N	2.60	0.69
1:H:39:MET:CE	1:H:275:GLY:HA3	2.22	0.69
1:L:25:PHE:HB3	1:L:60:ILE:HG12	1.75	0.69
1:L:42:GLU:OE1	1:L:45:LYS:HD3	1.93	0.69
1:G:19:LEU:HD21	1:I:53:VAL:HG11	1.73	0.69
1:I:221:ALA:HA	1:I:274:ASP:HB2	1.75	0.69
1:J:6:ASP:O	1:J:9:ALA:HB3	1.92	0.69
1:L:237:GLU:HA	1:L:240:ASN:HD21	1.57	0.69
1:E:287:THR:CG2	1:E:288:ASP:N	2.55	0.69
1:F:89:MET:HE3	1:F:156:ILE:HG21	1.73	0.69
1:I:29:THR:HG22	1:I:61:ASN:HB2	1.74	0.69
1:K:172:MET:HE1	1:L:173:LEU:HA	1.72	0.69
1:A:243:ILE:HG12	1:A:248:ILE:HD12	1.73	0.69
1:B:71:GLN:HG2	1:B:107:GLN:HE22	1.58	0.69
1:C:66:HIS:O	1:C:184:PRO:HD3	1.93	0.69
1:J:69:GLY:N	1:J:70:PRO:HD3	2.08	0.69
1:H:25:PHE:HA	1:H:28:LYS:CG	2.22	0.69
1:F:236:THR:CG2	1:F:237:GLU:N	2.56	0.69
1:E:212:GLU:O	1:E:268:THR:HB	1.93	0.68
1:F:231:LEU:O	1:F:232:THR:HB	1.93	0.68
1:H:213:LYS:HD3	1:H:269:SER:OG	1.93	0.68
1:L:44:LEU:HD22	1:L:278:PRO:HA	1.74	0.68
1:C:226:LYS:HG2	1:C:247:THR:HB	1.75	0.68
1:E:287:THR:CG2	1:E:289:SER:N	2.56	0.68
1:H:19:LEU:O	1:H:23:ARG:HG2	1.93	0.68
1:I:141:VAL:O	1:I:153:ILE:HG23	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:100:VAL:HG11	1:K:195:ASN:ND2	2.07	0.68
1:C:97:MET:HE1	1:C:195:ASN:HB2	1.74	0.68
1:E:287:THR:CG2	1:E:289:SER:H	2.01	0.68
1:I:72:ILE:HG22	1:I:76:LEU:HD12	1.75	0.68
1:J:92:THR:HG21	1:J:97:MET:SD	2.33	0.68
1:B:101:GLU:HA	1:B:185:ILE:HD13	1.76	0.68
1:I:60:ILE:O	1:I:62:PRO:HD3	1.93	0.68
1:C:215:MET:SD	1:C:281:VAL:HG23	2.33	0.68
1:H:262:ALA:O	1:H:267:VAL:HG23	1.93	0.68
1:K:124:ILE:HD12	1:K:173:LEU:CD2	2.18	0.68
1:L:274:ASP:OD1	1:L:276:ARG:HD2	1.93	0.68
1:D:252:MET:HE1	1:D:272:ILE:HD13	1.76	0.68
1:I:81:ILE:HG21	1:I:96:THR:CG2	2.24	0.68
1:J:36:GLY:N	1:J:68:GLY:HA3	2.08	0.68
1:K:159:VAL:HA	1:K:195:ASN:O	1.93	0.68
1:L:236:THR:HB	1:L:237:GLU:OE2	1.93	0.68
1:B:97:MET:HE1	1:B:194:TYR:C	2.13	0.68
1:E:35:GLY:HA2	1:E:39:MET:HG3	1.74	0.68
1:G:86:ILE:CG2	1:G:87:ASP:H	2.07	0.68
1:G:8:ALA:HB2	1:I:287:THR:CG2	2.24	0.68
1:J:282:LEU:O	1:J:286:PHE:HD1	1.77	0.68
1:J:15:LEU:CD1	1:K:15:LEU:HD21	2.22	0.68
1:L:68:GLY:CA	1:L:104:LEU:HD21	2.23	0.68
1:E:95:ALA:O	1:E:99:VAL:HG23	1.94	0.67
1:G:89:MET:HB3	2:G:1301:NLG:H8C2	1.76	0.67
1:I:65:VAL:HG21	1:I:202:ALA:HA	1.77	0.67
1:J:188:GLY:HA3	1:J:192:GLU:OE2	1.94	0.67
1:J:2:THR:HG22	1:J:3:LEU:N	2.09	0.67
1:F:133:LEU:HD21	1:F:182:ILE:CG2	2.23	0.67
1:F:271:HIS:NE2	1:F:294:LEU:HD12	2.10	0.67
1:G:253:LEU:HB2	1:G:254:PRO:CD	2.19	0.67
1:H:33:LYS:CB	1:H:216:LEU:HD12	2.24	0.67
1:A:224:MET:HA	1:A:229:GLN:O	1.94	0.67
1:G:69:GLY:O	1:G:72:ILE:HG13	1.93	0.67
1:J:220:ILE:CD1	3:J:1298:ADP:O3'	2.41	0.67
1:L:49:ALA:HB2	1:L:115:LEU:HG	1.76	0.67
1:E:50:ARG:HB2	1:E:119:HIS:ND1	2.10	0.67
1:E:19:LEU:HD23	1:E:22:ILE:HD11	1.77	0.67
1:E:287:THR:HG23	1:E:288:ASP:H	1.59	0.67
1:J:232:THR:O	1:J:234:LEU:HD23	1.95	0.67
1:C:248:ILE:HD13	1:C:256:ILE:CD1	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:129:LYS:HG2	1:D:187:VAL:HG22	1.77	0.67
1:L:66:HIS:CE1	1:L:183:ALA:CA	2.72	0.67
1:E:34:TYR:CG	1:E:35:GLY:N	2.61	0.67
1:F:271:HIS:HB3	1:F:273:ILE:CD1	2.24	0.67
1:I:256:ILE:HG22	1:I:260:LEU:CD1	2.25	0.67
1:K:129:LYS:HA	1:K:187:VAL:HG21	1.76	0.67
1:D:127:THR:HG22	1:D:183:ALA:HB3	1.77	0.67
1:G:248:ILE:HG21	1:G:256:ILE:HD12	1.77	0.67
1:G:257:ARG:O	1:G:260:LEU:HB3	1.95	0.67
1:L:68:GLY:HA3	1:L:104:LEU:HD21	1.75	0.67
1:B:15:LEU:HD21	1:C:15:LEU:HD22	1.76	0.67
1:H:90:ARG:HB3	2:H:1299:NLG:C8	2.24	0.67
1:K:72:ILE:HA	1:K:103:VAL:HG21	1.75	0.67
1:G:56:LYS:HA	1:G:60:ILE:O	1.95	0.67
1:G:9:ALA:HA	1:I:283:LEU:HD21	1.75	0.67
1:B:68:GLY:O	1:B:70:PRO:HD2	1.95	0.66
1:G:118:ARG:HG2	1:G:118:ARG:HH11	1.60	0.66
1:B:34:TYR:HD2	1:B:39:MET:CE	2.08	0.66
1:G:248:ILE:HD13	1:G:256:ILE:CD1	2.25	0.66
1:H:23:ARG:NH1	1:H:23:ARG:HG3	2.03	0.66
1:H:97:MET:CE	1:H:195:ASN:HB2	2.25	0.66
1:G:86:ILE:CG2	1:G:87:ASP:N	2.58	0.66
1:K:66:HIS:O	1:K:184:PRO:CG	2.43	0.66
1:A:143:ARG:CB	1:A:154:ILE:HD13	2.26	0.66
1:H:128:GLY:HA3	1:H:185:ILE:O	1.94	0.66
1:I:5:ARG:HD3	1:I:5:ARG:H	1.59	0.66
1:J:230:VAL:HG11	1:J:292:GLY:HA2	1.77	0.66
1:J:30:LEU:HD22	1:J:215:MET:CE	2.24	0.66
1:L:84:HIS:CE1	1:L:91:VAL:HG11	2.31	0.66
1:G:39:MET:HA	1:G:39:MET:CE	2.25	0.66
1:I:117:ASN:HD21	1:I:123:ALA:CB	2.08	0.66
1:K:195:ASN:HB3	2:K:1298:NLG:H8C1	1.77	0.66
1:C:223:LEU:C	1:C:223:LEU:HD12	2.15	0.66
1:L:223:LEU:O	1:L:230:VAL:HA	1.95	0.66
1:F:33:LYS:HD2	1:F:199:ASP:OD1	1.96	0.66
1:G:86:ILE:CB	1:G:91:VAL:HG23	2.18	0.66
1:J:15:LEU:HD13	1:K:15:LEU:CD1	2.26	0.66
1:A:223:LEU:HD12	1:A:224:MET:H	1.61	0.66
1:C:172:MET:HG2	1:D:172:MET:CE	2.26	0.66
1:E:72:ILE:HD11	1:E:104:LEU:HG	1.77	0.66
1:I:56:LYS:HE3	1:I:177:ASP:OD1	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:117:ASN:HA	1:J:121:GLY:O	1.95	0.66
1:J:54:LEU:HD23	1:J:282:LEU:CD1	2.21	0.66
1:F:213:LYS:HE3	1:F:271:HIS:NE2	2.11	0.66
1:J:100:VAL:HG11	1:J:195:ASN:HD21	1.61	0.66
1:A:4:SER:O	1:A:7:ASP:HB2	1.96	0.65
1:C:71:GLN:CD	1:C:71:GLN:H	1.99	0.65
1:J:285:ILE:HG22	1:J:286:PHE:HD1	1.57	0.65
1:A:282:LEU:O	1:A:286:PHE:HB2	1.95	0.65
1:D:143:ARG:HB2	1:D:154:ILE:CD1	2.26	0.65
1:D:248:ILE:HG21	1:D:256:ILE:HD12	1.78	0.65
1:J:282:LEU:O	1:J:286:PHE:CD1	2.50	0.65
1:L:252:MET:HE3	1:L:255:LYS:HB3	1.78	0.65
1:G:252:MET:HE3	1:G:256:ILE:HG13	1.77	0.65
1:A:86:ILE:HD12	1:A:156:ILE:CD1	2.26	0.65
1:B:34:TYR:HE1	1:B:48:PHE:HB2	1.61	0.65
1:F:223:LEU:HB3	1:F:293:THR:HG21	1.78	0.65
1:I:176:GLY:HA3	1:J:172:MET:HE1	1.77	0.65
1:J:31:VAL:HG21	1:J:206:ALA:HA	1.78	0.65
1:K:109:ASN:ND2	1:K:109:ASN:C	2.44	0.65
1:K:232:THR:CG2	1:K:294:LEU:HB3	2.26	0.65
1:B:129:LYS:HD3	1:B:187:VAL:CG1	2.26	0.65
1:B:50:ARG:CZ	1:C:12:ALA:HB1	2.26	0.65
1:B:213:LYS:HB2	1:B:269:SER:OG	1.97	0.65
1:G:118:ARG:HH11	1:G:118:ARG:CG	2.08	0.65
1:J:137:LYS:CG	1:J:138:LYS:N	2.60	0.65
1:B:137:LYS:HE3	1:B:161:GLU:OE2	1.97	0.65
1:B:239:VAL:HG13	1:B:256:ILE:HD12	1.78	0.65
1:E:33:LYS:HD3	1:E:34:TYR:O	1.97	0.65
1:G:33:LYS:O	1:G:217:LEU:HB2	1.96	0.65
1:H:86:ILE:HG22	1:H:87:ASP:N	2.12	0.65
1:J:3:LEU:HD22	1:K:21:TYR:HE2	1.55	0.65
1:K:71:GLN:HB3	1:K:107:GLN:HE22	1.57	0.65
1:G:142:THR:HG23	1:G:143:ARG:H	1.60	0.65
1:L:41:SER:OG	1:L:42:GLU:N	2.29	0.65
1:B:33:LYS:HE3	1:B:199:ASP:OD2	1.97	0.65
1:D:162:VAL:HB	1:D:204:LYS:HG3	1.79	0.65
1:H:232:THR:HG23	1:H:294:LEU:HB3	1.77	0.65
1:J:35:GLY:O	1:J:39:MET:SD	2.55	0.65
1:K:72:ILE:CA	1:K:103:VAL:HG11	2.27	0.65
1:D:14:VAL:CG1	1:F:11:VAL:HG21	2.19	0.64
1:F:233:GLY:HA2	1:F:294:LEU:HD23	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:112:ILE:O	1:H:116:ILE:HG13	1.96	0.64
1:H:19:LEU:O	1:H:23:ARG:CG	2.44	0.64
1:L:224:MET:HA	1:L:229:GLN:O	1.97	0.64
1:E:58:VAL:HG12	1:E:58:VAL:O	1.95	0.64
1:F:66:HIS:O	1:F:184:PRO:HD3	1.96	0.64
1:J:282:LEU:HD23	1:K:12:ALA:HB1	1.79	0.64
1:F:252:MET:O	1:F:256:ILE:HD12	1.96	0.64
1:F:273:ILE:HD11	1:F:284:GLU:HG2	1.79	0.64
1:H:273:ILE:HG22	1:H:274:ASP:N	2.11	0.64
1:D:101:GLU:HA	1:D:185:ILE:CD1	2.28	0.64
1:F:277:VAL:HB	1:F:280:ALA:HB2	1.78	0.64
1:G:232:THR:HG23	1:G:294:LEU:H	1.62	0.64
1:K:127:THR:HG22	1:K:183:ALA:CB	2.20	0.64
1:K:24:ARG:HD2	1:K:25:PHE:CE2	2.32	0.64
1:G:71:GLN:HG3	1:G:108:VAL:HG21	1.79	0.64
1:A:36:GLY:C	1:A:38:ALA:N	2.49	0.64
1:B:199:ASP:HB3	1:B:258:CYS:SG	2.38	0.64
1:B:34:TYR:HD2	1:B:39:MET:HE3	1.63	0.64
1:B:287:THR:CG2	1:B:288:ASP:H	2.10	0.64
1:B:58:VAL:O	1:B:58:VAL:HG13	1.97	0.64
1:D:75:LEU:HD23	1:D:99:VAL:HG13	1.79	0.64
1:F:236:THR:HG22	1:F:237:GLU:H	1.61	0.64
1:L:30:LEU:HD13	1:L:215:MET:CE	2.27	0.64
1:A:268:THR:O	1:A:296:SER:HB2	1.98	0.64
1:C:87:ASP:OD2	1:C:144:GLN:HG2	1.97	0.64
1:B:35:GLY:CA	1:B:39:MET:HE3	2.27	0.64
1:C:220:ILE:O	1:C:220:ILE:HG13	1.98	0.64
1:F:11:VAL:HG13	1:F:15:LEU:CD1	2.28	0.64
1:F:273:ILE:CD1	1:F:284:GLU:HG2	2.28	0.64
1:G:236:THR:HG22	1:G:240:ASN:HD21	1.61	0.64
1:H:252:MET:O	1:H:256:ILE:HG12	1.97	0.64
1:I:58:VAL:HG12	1:I:58:VAL:O	1.98	0.64
1:K:179:ILE:HG22	1:K:179:ILE:O	1.97	0.64
1:K:76:LEU:CD2	1:K:99:VAL:HG11	2.27	0.64
1:L:54:LEU:HD23	1:L:282:LEU:HD21	1.79	0.64
1:B:287:THR:CG2	1:B:288:ASP:N	2.60	0.63
1:D:248:ILE:HD13	1:D:256:ILE:HD13	1.78	0.63
1:I:81:ILE:CG2	1:I:82:GLU:N	2.61	0.63
1:I:81:ILE:HG22	1:I:82:GLU:N	2.12	0.63
1:K:173:LEU:HD22	1:K:178:PHE:CB	2.28	0.63
1:A:117:ASN:HD21	1:A:123:ALA:N	1.94	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:15:LEU:HB2	1:K:15:LEU:HD21	1.78	0.63
1:K:196:ILE:CG2	1:K:200:LEU:CD2	2.76	0.63
1:K:33:LYS:HA	1:K:65:VAL:O	1.98	0.63
1:A:101:GLU:CG	1:A:185:ILE:HD13	2.28	0.63
1:F:219:ASN:HD22	1:F:219:ASN:C	2.02	0.63
1:F:37:ASN:HD22	1:F:37:ASN:N	1.97	0.63
1:H:239:VAL:O	1:H:243:ILE:HG12	1.98	0.63
1:I:93:ASP:CG	1:I:96:THR:HG23	2.17	0.63
1:J:249:TYR:CD1	1:J:250:GLY:N	2.64	0.63
1:E:117:ASN:ND2	1:E:122:SER:HA	2.14	0.63
1:I:273:ILE:HD13	1:I:284:GLU:CG	2.25	0.63
1:I:38:ALA:HB3	1:I:219:ASN:OD1	1.98	0.63
1:I:55:MET:HE3	1:I:285:ILE:HD11	1.78	0.63
1:A:97:MET:HE1	1:A:195:ASN:CB	2.27	0.63
1:C:28:LYS:HG3	1:C:29:THR:N	2.14	0.63
1:H:39:MET:CE	1:H:217:LEU:HD23	2.29	0.63
1:H:97:MET:HE3	1:H:195:ASN:HB2	1.78	0.63
1:I:75:LEU:HD22	1:I:103:VAL:HG23	1.81	0.63
1:I:154:ILE:HG22	1:I:156:ILE:HG13	1.81	0.63
1:I:242:LEU:HA	1:I:245:ASP:OD1	1.98	0.63
1:A:23:ARG:NH1	1:A:23:ARG:HG2	2.11	0.63
1:E:16:SER:O	1:E:19:LEU:HB2	1.98	0.63
1:E:29:THR:O	1:E:211:ALA:HB1	1.99	0.63
1:F:142:THR:CG2	1:F:151:PRO:HB3	2.29	0.63
1:F:22:ILE:HG21	1:F:58:VAL:HG13	1.80	0.63
1:H:196:ILE:HG22	1:H:197:ASN:N	2.13	0.63
1:I:117:ASN:HD21	1:I:123:ALA:HB3	1.62	0.63
1:I:92:THR:HG22	1:I:96:THR:OG1	1.99	0.63
1:L:33:LYS:HA	1:L:65:VAL:O	1.99	0.63
1:E:39:MET:HE1	1:E:68:GLY:HA2	1.81	0.63
1:I:117:ASN:ND2	1:I:123:ALA:HB3	2.14	0.63
1:J:33:LYS:HE2	1:J:34:TYR:O	1.99	0.63
1:L:22:ILE:HD11	1:L:286:PHE:CE1	2.34	0.63
1:E:36:GLY:HA3	3:E:1299:ADP:O2B	1.99	0.63
1:K:196:ILE:HG21	1:K:200:LEU:CD2	2.29	0.63
1:F:252:MET:HG3	1:F:256:ILE:CD1	2.29	0.62
1:G:207:GLU:O	1:G:210:LYS:HD3	1.98	0.62
1:H:11:VAL:O	1:H:15:LEU:HG	1.99	0.62
1:D:252:MET:O	1:D:256:ILE:HG13	1.98	0.62
1:D:296:SER:OG	1:D:299:LYS:HB3	1.98	0.62
1:H:199:ASP:OD1	1:H:216:LEU:HD11	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:225:ASP:HB3	1:H:231:LEU:HD21	1.79	0.62
1:I:34:TYR:CG	1:I:35:GLY:N	2.66	0.62
1:K:29:THR:HG22	1:K:61:ASN:HB2	1.81	0.62
1:B:34:TYR:CD2	1:B:39:MET:CE	2.83	0.62
1:K:232:THR:HG23	1:K:294:LEU:CB	2.29	0.62
1:A:10:GLN:NE2	1:E:10:GLN:HG3	2.14	0.62
1:A:162:VAL:HB	1:A:204:LYS:HD2	1.80	0.62
1:D:218:THR:HG23	1:D:220:ILE:H	1.65	0.62
1:K:124:ILE:HG22	1:K:126:LEU:CD1	2.29	0.62
1:L:82:GLU:HG3	1:L:83:SER:N	2.15	0.62
1:B:252:MET:HE3	1:B:255:LYS:HB3	1.79	0.62
1:B:49:ALA:HB2	1:B:115:LEU:HB3	1.81	0.62
1:L:143:ARG:HH21	1:L:153:ILE:HD11	1.64	0.62
1:C:36:GLY:O	1:C:40:GLU:HG2	1.99	0.62
1:I:162:VAL:HB	1:I:204:LYS:HG3	1.82	0.62
1:J:219:ASN:ND2	3:J:1298:ADP:O3'	2.28	0.62
1:H:22:ILE:HD11	1:H:286:PHE:HE2	1.62	0.62
1:L:140:THR:HG22	1:L:153:ILE:CD1	2.29	0.62
1:L:223:LEU:HD11	1:L:248:ILE:CD1	2.28	0.62
1:B:223:LEU:HD11	1:B:248:ILE:HG12	1.81	0.62
1:F:196:ILE:HG22	1:F:197:ASN:H	1.63	0.62
1:I:223:LEU:HD12	1:I:224:MET:N	2.15	0.62
1:J:218:THR:HG23	1:J:220:ILE:H	1.65	0.62
1:K:107:GLN:HG3	1:K:108:VAL:N	2.15	0.62
1:K:18:ALA:O	1:K:22:ILE:HG13	2.00	0.62
1:K:271:HIS:ND1	1:K:284:GLU:HG3	2.15	0.62
1:B:34:TYR:CE1	1:B:48:PHE:CB	2.83	0.62
1:I:28:LYS:HB3	1:I:212:GLU:HB2	1.82	0.62
1:I:69:GLY:N	1:I:70:PRO:HD2	2.14	0.62
1:J:219:ASN:ND2	1:J:219:ASN:C	2.49	0.62
1:K:129:LYS:HZ3	1:K:187:VAL:HG11	1.64	0.62
1:I:232:THR:HG23	1:I:294:LEU:H	1.64	0.62
1:J:137:LYS:CG	1:J:138:LYS:H	2.13	0.62
1:J:25:PHE:HD2	1:J:212:GLU:HG2	1.64	0.62
1:K:263:VAL:HG21	1:K:296:SER:O	2.00	0.62
1:A:86:ILE:HG22	1:A:87:ASP:N	2.15	0.61
1:D:217:LEU:N	1:D:217:LEU:HD23	2.16	0.61
1:F:138:LYS:CE	1:F:157:GLY:HA3	2.24	0.61
1:E:251:GLY:HA3	3:E:1299:ADP:O2A	1.99	0.61
1:G:32:ILE:HD11	1:G:55:MET:CE	2.30	0.61
1:H:69:GLY:H	1:H:70:PRO:HD3	1.61	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:30:LEU:HD22	1:I:213:LYS:HB3	1.82	0.61
1:K:271:HIS:CD2	1:K:294:LEU:HD12	2.35	0.61
1:K:72:ILE:HA	1:K:103:VAL:HG11	1.81	0.61
1:L:252:MET:HG3	1:L:252:MET:O	1.99	0.61
1:D:285:ILE:HG22	1:D:286:PHE:N	2.14	0.61
1:E:21:TYR:O	1:E:24:ARG:HG3	2.00	0.61
1:G:252:MET:HE1	1:G:255:LYS:HD2	1.82	0.61
1:G:86:ILE:HG22	1:G:87:ASP:N	2.11	0.61
1:I:100:VAL:HG11	1:I:195:ASN:OD1	2.01	0.61
1:J:248:ILE:HD13	1:J:256:ILE:CD1	2.30	0.61
1:J:34:TYR:CD2	1:J:35:GLY:N	2.68	0.61
1:I:23:ARG:HH11	1:I:23:ARG:HG2	1.65	0.61
1:J:30:LEU:HD12	1:J:60:ILE:HG21	1.80	0.61
1:H:19:LEU:HD21	1:L:53:VAL:HG11	1.81	0.61
1:L:73:GLY:HA2	1:L:76:LEU:HD12	1.83	0.61
1:G:156:ILE:O	1:G:156:ILE:HG22	2.01	0.61
1:J:124:ILE:HG23	1:J:126:LEU:HD21	1.81	0.61
1:K:129:LYS:CD	1:K:187:VAL:HG22	2.29	0.61
1:A:243:ILE:HD11	1:A:256:ILE:HG21	1.83	0.61
1:C:65:VAL:HG21	1:C:202:ALA:HA	1.83	0.61
1:D:57:ALA:CB	1:F:19:LEU:HD21	2.31	0.61
1:F:221:ALA:HA	1:F:274:ASP:HB2	1.83	0.61
1:G:101:GLU:HA	1:G:185:ILE:CD1	2.31	0.61
1:H:217:LEU:HG	1:H:275:GLY:HA3	1.83	0.61
1:H:54:LEU:O	1:H:58:VAL:HG23	2.00	0.61
1:J:15:LEU:HD12	1:K:15:LEU:HD11	1.83	0.61
1:K:196:ILE:HG21	1:K:200:LEU:HD22	1.82	0.61
1:K:273:ILE:CG2	1:K:274:ASP:H	2.10	0.61
1:D:30:LEU:HD12	1:D:55:MET:HE3	1.82	0.61
1:G:78:ARG:HG3	1:H:79:LEU:HD11	1.82	0.61
1:I:78:ARG:HG2	1:J:79:LEU:CD1	2.31	0.61
1:B:25:PHE:HD2	1:B:212:GLU:HG2	1.66	0.60
1:D:225:ASP:OD1	1:D:231:LEU:HD21	2.01	0.60
1:D:30:LEU:HD12	1:D:55:MET:CE	2.31	0.60
1:B:104:LEU:HD13	1:B:184:PRO:HD2	1.84	0.60
1:F:3:LEU:HD21	1:F:8:ALA:HA	1.83	0.60
1:L:143:ARG:N	1:L:143:ARG:HD2	2.14	0.60
1:E:37:ASN:C	1:E:219:ASN:HD21	2.04	0.60
1:B:167:VAL:HG23	1:B:171:ASN:ND2	2.15	0.60
1:F:139:LEU:CD1	1:F:161:GLU:HG2	2.30	0.60
1:F:140:THR:HG23	1:F:153:ILE:HD13	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:255:LYS:HA	1:H:258:CYS:SG	2.40	0.60
1:B:11:VAL:HG21	1:C:14:VAL:HG12	1.83	0.60
1:D:253:LEU:HB3	1:D:254:PRO:CD	2.31	0.60
1:G:142:THR:HG22	1:G:143:ARG:N	2.16	0.60
1:K:21:TYR:HB3	1:K:286:PHE:O	2.02	0.60
1:A:200:LEU:HD23	1:A:200:LEU:N	2.16	0.60
1:H:85:PHE:O	1:H:86:ILE:CG1	2.45	0.60
1:H:90:ARG:HG3	1:H:90:ARG:HH11	1.66	0.60
1:J:131:ALA:HB3	1:J:169:LEU:HD22	1.84	0.60
1:J:220:ILE:CD1	3:J:1298:ADP:C2'	2.79	0.60
1:K:79:LEU:CD2	1:L:79:LEU:CD2	2.68	0.60
1:A:273:ILE:HD11	1:A:284:GLU:HG2	1.83	0.60
1:A:51:ASP:CG	1:A:282:LEU:HG	2.22	0.60
1:D:271:HIS:CE1	1:D:284:GLU:HG2	2.37	0.60
1:B:175:LYS:O	1:B:175:LYS:HG3	2.02	0.60
1:F:142:THR:HG21	1:F:151:PRO:HB3	1.82	0.60
1:K:273:ILE:CG2	1:K:274:ASP:N	2.64	0.60
1:L:100:VAL:HG12	1:L:104:LEU:HD12	1.82	0.60
1:D:235:SER:OG	1:D:238:GLN:HG3	2.01	0.60
1:F:70:PRO:HD2	1:F:71:GLN:OE1	2.02	0.60
1:G:232:THR:HG22	1:G:233:GLY:N	2.17	0.60
1:E:101:GLU:HA	1:E:185:ILE:CD1	2.32	0.60
1:F:30:LEU:HD12	1:F:55:MET:HE1	1.84	0.60
1:G:273:ILE:HD13	1:G:291:VAL:O	2.02	0.60
1:J:284:GLU:OE2	1:J:291:VAL:HG22	2.02	0.60
1:D:66:HIS:O	1:D:184:PRO:HD3	2.01	0.59
1:J:23:ARG:HH21	1:K:53:VAL:HG12	1.66	0.59
1:J:248:ILE:HG22	1:J:253:LEU:HD23	1.84	0.59
1:J:37:ASN:O	1:J:40:GLU:CG	2.50	0.59
1:A:101:GLU:HA	1:A:185:ILE:HD11	1.84	0.59
1:A:22:ILE:CG2	1:A:58:VAL:HG13	2.23	0.59
1:D:253:LEU:CB	1:D:254:PRO:HD3	2.32	0.59
1:F:139:LEU:CD1	1:F:161:GLU:CG	2.80	0.59
1:K:72:ILE:HG13	1:K:103:VAL:HG11	1.85	0.59
1:F:126:LEU:O	1:F:182:ILE:HA	2.01	0.59
1:H:259:ALA:O	1:H:263:VAL:HG23	2.02	0.59
1:C:297:ASN:O	1:C:298:ARG:HB2	2.02	0.59
1:G:39:MET:HA	1:G:39:MET:HE3	1.84	0.59
1:I:69:GLY:N	1:I:70:PRO:CD	2.65	0.59
1:L:33:LYS:HE2	1:L:199:ASP:OD1	2.03	0.59
1:A:74:ASP:O	1:A:77:LYS:HG2	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:273:ILE:HG12	1:C:274:ASP:N	2.17	0.59
1:C:291:VAL:O	1:C:291:VAL:HG23	2.03	0.59
1:F:244:ALA:C	1:F:246:GLY:N	2.55	0.59
1:H:221:ALA:HA	1:H:274:ASP:HB2	1.85	0.59
1:J:113:VAL:HG13	1:J:123:ALA:HB3	1.84	0.59
1:A:242:LEU:O	1:A:242:LEU:HD12	2.02	0.59
1:C:101:GLU:HG3	1:C:185:ILE:HD13	1.84	0.59
1:E:34:TYR:HD1	1:E:217:LEU:HD12	1.66	0.59
1:H:22:ILE:HD11	1:H:286:PHE:CD2	2.37	0.59
1:J:66:HIS:NE2	1:J:109:ASN:HA	2.18	0.59
1:J:118:ARG:HH11	1:J:118:ARG:HG3	1.67	0.59
1:L:66:HIS:HE1	1:L:183:ALA:HA	1.62	0.59
1:B:143:ARG:HG2	1:B:154:ILE:CD1	2.33	0.59
1:E:101:GLU:HA	1:E:185:ILE:HD11	1.84	0.59
1:G:255:LYS:O	1:G:258:CYS:HB3	2.03	0.59
1:I:86:ILE:O	1:I:86:ILE:HG23	2.03	0.59
1:J:248:ILE:CD1	1:J:256:ILE:HD12	2.32	0.59
1:K:31:VAL:HG21	1:K:206:ALA:HA	1.85	0.59
1:K:72:ILE:HG13	1:K:103:VAL:CG1	2.32	0.59
1:B:57:ALA:CB	1:C:19:LEU:HD21	2.32	0.59
1:D:252:MET:CE	1:D:255:LYS:HB3	2.32	0.59
1:D:248:ILE:HG21	1:D:256:ILE:HD11	1.85	0.59
1:E:10:GLN:HG2	1:E:11:VAL:H	1.65	0.59
1:F:271:HIS:ND1	1:F:284:GLU:CG	2.65	0.59
1:I:262:ALA:O	1:I:267:VAL:HB	2.03	0.59
1:A:139:LEU:H	1:A:160:GLY:HA2	1.68	0.58
1:C:217:LEU:HD22	1:C:273:ILE:CG2	2.33	0.58
1:E:24:ARG:HD2	1:E:25:PHE:CZ	2.38	0.58
1:F:24:ARG:HH21	1:F:288:ASP:HB2	1.68	0.58
1:F:97:MET:CE	1:F:195:ASN:HB2	2.32	0.58
1:J:12:ALA:CB	1:K:282:LEU:HD13	2.32	0.58
1:K:24:ARG:HH12	1:K:288:ASP:HA	1.68	0.58
1:K:97:MET:CE	1:K:195:ASN:HB2	2.33	0.58
1:K:75:LEU:HD22	1:L:102:MET:SD	2.43	0.58
1:C:285:ILE:HG13	1:C:286:PHE:CD1	2.38	0.58
1:G:232:THR:HG23	1:G:294:LEU:HB3	1.85	0.58
1:G:2:THR:O	1:G:2:THR:HG22	2.03	0.58
1:H:34:TYR:HD2	1:H:35:GLY:H	1.50	0.58
1:H:97:MET:HA	1:H:97:MET:CE	2.32	0.58
1:L:162:VAL:CB	1:L:204:LYS:HG3	2.33	0.58
1:L:271:HIS:CD2	1:L:284:GLU:HG2	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:3:LEU:CD2	1:K:21:TYR:CE2	2.83	0.58
1:K:279:ASN:HB3	1:K:282:LEU:HD12	1.84	0.58
1:E:117:ASN:HD21	1:E:123:ALA:H	1.50	0.58
1:G:142:THR:O	1:G:143:ARG:CB	2.51	0.58
1:J:207:GLU:OE2	1:J:262:ALA:HA	2.03	0.58
1:J:35:GLY:O	1:J:39:MET:HE3	2.01	0.58
1:K:47:GLY:O	1:K:50:ARG:HG2	2.03	0.58
1:K:53:VAL:O	1:K:56:LYS:HB3	2.04	0.58
1:A:42:GLU:O	1:A:45:LYS:HB2	2.04	0.58
1:E:127:THR:HG22	1:E:183:ALA:HB3	1.86	0.58
1:E:66:HIS:O	1:E:184:PRO:HD3	2.02	0.58
1:E:58:VAL:CG1	1:E:58:VAL:O	2.50	0.58
1:H:232:THR:CG2	1:H:294:LEU:HB3	2.34	0.58
1:J:54:LEU:CD2	1:J:282:LEU:HD13	2.24	0.58
1:L:55:MET:SD	1:L:285:ILE:HG13	2.44	0.58
1:B:34:TYR:HH	1:B:45:LYS:HA	1.68	0.58
1:B:52:VAL:HA	1:B:55:MET:HE3	1.86	0.58
1:B:72:ILE:HD11	1:B:104:LEU:HG	1.85	0.58
1:D:291:VAL:O	1:D:291:VAL:HG12	2.03	0.58
1:F:89:MET:HE3	1:F:156:ILE:CG2	2.34	0.58
1:F:30:LEU:HD12	1:F:55:MET:CE	2.34	0.58
1:J:211:ALA:O	1:J:267:VAL:HG13	2.04	0.58
1:K:53:VAL:HG11	1:K:119:HIS:O	2.04	0.58
1:H:287:THR:HG23	1:L:3:LEU:HB3	1.83	0.58
1:L:85:PHE:CD2	1:L:89:MET:O	2.52	0.58
1:D:143:ARG:HB2	1:D:154:ILE:HD11	1.86	0.58
1:A:273:ILE:CG2	1:A:274:ASP:N	2.67	0.58
1:E:287:THR:CG2	1:E:288:ASP:H	2.17	0.58
1:G:195:ASN:ND2	2:G:1301:NLG:H8C1	2.19	0.58
1:H:90:ARG:HG2	1:H:91:VAL:O	2.03	0.58
1:I:90:ARG:O	1:I:159:VAL:HG21	2.04	0.58
1:L:55:MET:HB2	1:L:62:PRO:HG3	1.86	0.58
1:D:197:ASN:HB3	1:D:200:LEU:HG	1.86	0.58
1:E:141:VAL:CG2	1:E:156:ILE:HD12	2.34	0.58
1:H:207:GLU:CG	1:H:262:ALA:HA	2.34	0.58
1:A:285:ILE:C	1:A:287:THR:H	2.08	0.58
1:H:254:PRO:O	1:H:258:CYS:SG	2.62	0.58
1:K:33:LYS:HE3	1:K:199:ASP:OD1	2.03	0.58
1:L:251:GLY:HA3	3:L:1300:ADP:O2A	2.03	0.58
1:J:33:LYS:HA	1:J:65:VAL:O	2.04	0.57
1:B:34:TYR:CE1	1:B:48:PHE:HB2	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:76:LEU:HD13	1:B:99:VAL:HG11	1.86	0.57
1:E:128:GLY:HA3	1:E:185:ILE:O	2.04	0.57
1:F:219:ASN:ND2	1:F:219:ASN:H	2.02	0.57
1:H:238:GLN:O	1:H:242:LEU:CG	2.50	0.57
1:I:48:PHE:O	1:I:52:VAL:HG23	2.04	0.57
1:E:34:TYR:OH	1:E:45:LYS:HA	2.04	0.57
1:H:38:ALA:HB2	1:H:219:ASN:HD22	1.69	0.57
1:H:270:ALA:O	1:H:295:ILE:HB	2.05	0.57
1:I:253:LEU:HB2	1:I:254:PRO:HD3	1.86	0.57
1:K:19:LEU:HB3	1:K:20:PRO:HD3	1.86	0.57
1:C:55:MET:HE2	1:C:285:ILE:HD13	1.87	0.57
1:H:39:MET:CE	1:H:217:LEU:HG	2.32	0.57
1:L:167:VAL:HG11	1:L:208:ALA:O	2.04	0.57
1:B:5:ARG:HG3	1:C:291:VAL:CG1	2.34	0.57
1:D:213:LYS:HZ3	1:D:271:HIS:CE1	2.22	0.57
1:E:93:ASP:OD1	1:E:93:ASP:N	2.36	0.57
1:E:97:MET:HE3	1:E:158:HIS:HB3	1.86	0.57
1:H:10:GLN:HG3	1:H:11:VAL:N	2.17	0.57
1:F:89:MET:CE	1:F:139:LEU:HD23	2.35	0.57
1:H:50:ARG:HG2	1:H:119:HIS:ND1	2.20	0.57
1:I:44:LEU:HD11	1:I:276:ARG:O	2.05	0.57
1:K:18:ALA:HA	1:K:21:TYR:CD1	2.39	0.57
1:L:113:VAL:HG12	1:L:114:ASN:N	2.18	0.57
1:F:242:LEU:HA	1:F:245:ASP:HB2	1.87	0.57
1:G:252:MET:HE1	1:G:272:ILE:CD1	2.34	0.57
1:H:19:LEU:HD21	1:L:53:VAL:CG1	2.33	0.57
1:J:33:LYS:C	1:J:33:LYS:HD3	2.25	0.57
1:K:259:ALA:HB1	1:K:295:ILE:HG21	1.85	0.57
1:D:220:ILE:O	1:D:221:ALA:CB	2.53	0.57
1:K:249:TYR:O	1:K:252:MET:HB3	2.05	0.57
1:B:75:LEU:HD23	1:B:99:VAL:HG13	1.87	0.57
1:C:225:ASP:OD2	1:C:229:GLN:HB3	2.04	0.57
1:E:291:VAL:HG23	1:E:292:GLY:N	2.20	0.57
1:G:206:ALA:O	1:G:210:LYS:N	2.37	0.57
1:I:117:ASN:ND2	1:I:123:ALA:N	2.45	0.57
1:I:56:LYS:CE	1:I:177:ASP:OD1	2.52	0.57
1:I:172:MET:HE1	1:J:176:GLY:HA3	1.87	0.57
1:F:11:VAL:HG13	1:F:15:LEU:HD11	1.87	0.57
1:J:162:VAL:HB	1:J:204:LYS:HG3	1.87	0.57
1:D:252:MET:HE1	1:D:255:LYS:HD2	1.87	0.56
1:F:11:VAL:HG13	1:F:15:LEU:HG	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:218:THR:HG23	1:H:220:ILE:O	2.05	0.56
1:I:55:MET:HE1	1:I:215:MET:HE1	1.85	0.56
1:J:232:THR:CG2	1:J:233:GLY:H	2.13	0.56
1:L:285:ILE:HG22	1:L:286:PHE:HD1	1.68	0.56
1:F:6:ASP:O	1:F:9:ALA:HB3	2.05	0.56
1:H:25:PHE:HB2	1:H:60:ILE:HD13	1.86	0.56
1:J:19:LEU:HD22	1:K:54:LEU:HD13	1.88	0.56
1:B:141:VAL:HG12	1:B:142:THR:N	2.20	0.56
1:C:23:ARG:HA	1:C:26:VAL:CG2	2.35	0.56
1:D:252:MET:CE	1:D:255:LYS:HD2	2.34	0.56
1:F:200:LEU:HD23	1:F:258:CYS:SG	2.45	0.56
1:J:209:LEU:O	1:J:210:LYS:C	2.42	0.56
1:B:34:TYR:CD1	1:B:48:PHE:CG	2.93	0.56
1:C:213:LYS:HD3	1:C:271:HIS:NE2	2.20	0.56
1:D:271:HIS:CD2	1:D:271:HIS:N	2.73	0.56
1:G:118:ARG:HG2	1:G:118:ARG:NH1	2.20	0.56
1:H:148:MET:HG3	1:H:148:MET:O	2.06	0.56
1:I:94:ALA:O	1:I:98:ASP:HB2	2.06	0.56
1:J:60:ILE:HD13	1:J:285:ILE:CD1	2.35	0.56
1:D:223:LEU:HD23	1:D:224:MET:N	2.21	0.56
1:E:167:VAL:HG12	1:E:171:ASN:HD21	1.66	0.56
1:E:35:GLY:CA	1:E:39:MET:HG3	2.36	0.56
1:G:89:MET:HB3	2:G:1301:NLG:C8	2.34	0.56
1:J:273:ILE:HG22	1:J:274:ASP:N	2.21	0.56
1:J:54:LEU:CD2	1:J:282:LEU:CD1	2.83	0.56
1:J:37:ASN:O	1:J:40:GLU:N	2.36	0.56
1:E:81:ILE:O	1:E:82:GLU:HB3	2.05	0.56
1:I:107:GLN:O	1:I:111:ASP:HB2	2.05	0.56
1:J:109:ASN:HD22	1:J:183:ALA:HB2	1.69	0.56
1:K:34:TYR:OH	1:K:45:LYS:HG2	2.06	0.56
1:E:141:VAL:HG21	1:E:156:ILE:HD12	1.86	0.56
1:F:196:ILE:CG2	1:F:197:ASN:H	2.18	0.56
1:F:200:LEU:O	1:F:204:LYS:HG2	2.06	0.56
1:L:156:ILE:CG2	1:L:159:VAL:HG21	2.34	0.56
1:A:39:MET:HE3	1:A:39:MET:H	1.70	0.56
1:B:253:LEU:HB2	1:B:254:PRO:HD3	1.86	0.56
1:B:294:LEU:HD23	1:B:294:LEU:C	2.26	0.56
1:B:34:TYR:HD1	1:B:48:PHE:CD1	2.22	0.56
1:G:72:ILE:HG21	1:G:100:VAL:HG22	1.87	0.56
1:E:139:LEU:N	1:E:160:GLY:HA2	2.21	0.56
1:F:143:ARG:HD2	1:F:154:ILE:HG13	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:86:ILE:CD1	1:G:91:VAL:CG2	2.76	0.56
1:I:79:LEU:CD1	1:J:78:ARG:HG2	2.35	0.56
1:J:200:LEU:HD23	1:J:258:CYS:SG	2.45	0.56
1:I:79:LEU:HD22	1:J:78:ARG:NE	2.21	0.56
1:K:34:TYR:CZ	1:K:37:ASN:HB2	2.40	0.56
1:A:235:SER:OG	1:A:238:GLN:HG3	2.06	0.56
1:A:234:LEU:O	1:A:295:ILE:HA	2.06	0.56
1:C:97:MET:CE	1:C:195:ASN:HB2	2.35	0.56
1:E:117:ASN:HD21	1:E:122:SER:HA	1.69	0.56
1:G:128:GLY:HA3	1:G:185:ILE:O	2.06	0.56
1:H:70:PRO:CD	1:H:71:GLN:OE1	2.52	0.56
1:L:136:ALA:O	1:L:188:GLY:HA2	2.06	0.56
1:L:131:ALA:HB3	1:L:169:LEU:HD22	1.87	0.56
1:D:212:GLU:O	1:D:268:THR:HB	2.05	0.56
1:D:243:ILE:HD13	1:D:243:ILE:C	2.26	0.56
1:H:7:ASP:O	1:H:11:VAL:HG23	2.06	0.56
1:K:273:ILE:HD11	1:K:284:GLU:CG	2.36	0.56
1:A:141:VAL:HG21	1:A:156:ILE:CG1	2.36	0.55
1:C:44:LEU:HD21	1:C:276:ARG:HA	1.87	0.55
1:G:86:ILE:CB	1:G:91:VAL:CG2	2.79	0.55
1:H:206:ALA:CB	1:H:214:LEU:HD22	2.36	0.55
1:C:37:ASN:O	1:I:249:TYR:CE2	2.59	0.55
1:K:162:VAL:HB	1:K:204:LYS:HG3	1.86	0.55
1:K:30:LEU:CD2	1:K:213:LYS:HB2	2.37	0.55
1:L:220:ILE:HG23	1:L:222:GLY:H	1.71	0.55
1:J:135:ARG:NH1	1:J:164:GLY:HA3	2.21	0.55
1:L:22:ILE:HD13	1:L:58:VAL:HG11	1.88	0.55
1:L:38:ALA:C	1:L:40:GLU:H	2.10	0.55
1:A:134:ILE:CG2	1:A:162:VAL:HG22	2.36	0.55
1:B:167:VAL:HG23	1:B:171:ASN:HD22	1.70	0.55
1:F:196:ILE:CG2	1:F:197:ASN:N	2.68	0.55
1:F:213:LYS:HE3	1:F:271:HIS:HE2	1.69	0.55
1:F:73:GLY:O	1:F:77:LYS:HD3	2.06	0.55
1:I:257:ARG:O	1:I:261:GLU:CG	2.54	0.55
1:J:38:ALA:C	1:J:40:GLU:H	2.10	0.55
1:E:22:ILE:HG22	1:E:286:PHE:CD1	2.42	0.55
1:F:199:ASP:OD2	1:F:255:LYS:HE3	2.07	0.55
1:G:34:TYR:HB2	1:G:48:PHE:CZ	2.42	0.55
1:I:8:ALA:HA	1:I:11:VAL:HB	1.87	0.55
1:B:248:ILE:HD13	1:B:256:ILE:CD1	2.36	0.55
1:E:218:THR:HG23	1:E:220:ILE:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:36:GLY:O	1:E:39:MET:HE3	2.07	0.55
1:F:101:GLU:HA	1:F:185:ILE:CD1	2.35	0.55
1:I:167:VAL:HG12	1:I:209:LEU:CD2	2.31	0.55
1:K:260:LEU:CD2	1:K:295:ILE:HD11	2.23	0.55
1:C:230:VAL:CG1	1:C:292:GLY:HA2	2.34	0.55
1:C:58:VAL:HG13	1:C:58:VAL:O	2.07	0.55
1:H:143:ARG:CD	1:H:154:ILE:HD11	2.36	0.55
1:J:5:ARG:O	1:J:8:ALA:N	2.36	0.55
1:K:21:TYR:HD1	1:K:21:TYR:H	1.55	0.55
1:L:30:LEU:HD13	1:L:215:MET:HE3	1.88	0.55
1:G:242:LEU:HD22	1:G:247:THR:HG21	1.88	0.55
1:H:271:HIS:CD2	1:H:271:HIS:N	2.75	0.55
1:J:269:SER:HB3	1:J:296:SER:OG	2.06	0.55
1:B:123:ALA:O	1:B:124:ILE:HD12	2.07	0.55
1:B:149:THR:CG2	1:B:150:LYS:N	2.70	0.55
1:E:291:VAL:CG2	1:E:292:GLY:N	2.70	0.55
1:H:39:MET:CE	1:H:217:LEU:CD2	2.82	0.55
1:K:126:LEU:O	1:K:182:ILE:HA	2.07	0.55
1:H:144:GLN:HG2	1:H:151:PRO:CG	2.34	0.55
1:H:225:ASP:HB3	1:H:231:LEU:HD11	1.89	0.55
1:G:11:VAL:HG12	1:I:286:PHE:CD2	2.41	0.55
1:J:28:LYS:HB3	1:J:212:GLU:HB2	1.88	0.55
1:K:12:ALA:O	1:K:16:SER:HB2	2.06	0.55
1:K:30:LEU:HD12	1:K:60:ILE:HG21	1.89	0.55
1:L:76:LEU:CD1	1:L:90:ARG:HH21	2.20	0.55
1:A:269:SER:HA	1:A:296:SER:HB3	1.89	0.55
1:B:143:ARG:CG	1:B:154:ILE:HG13	2.37	0.55
1:G:205:VAL:O	1:G:209:LEU:HB2	2.07	0.55
1:I:176:GLY:HA3	1:J:172:MET:CE	2.37	0.55
1:K:72:ILE:N	1:K:103:VAL:HG11	2.22	0.55
1:B:253:LEU:CB	1:B:254:PRO:HD3	2.38	0.54
1:H:81:ILE:HG22	1:H:82:GLU:O	2.07	0.54
1:A:128:GLY:HA3	1:A:185:ILE:O	2.06	0.54
1:B:252:MET:HE3	1:B:255:LYS:CB	2.37	0.54
1:C:146:PRO:HD2	1:C:149:THR:HB	1.89	0.54
1:C:16:SER:HA	1:C:19:LEU:HD12	1.89	0.54
1:I:86:ILE:HG21	1:I:156:ILE:HG12	1.88	0.54
1:K:13:LYS:O	1:K:17:GLU:HG3	2.06	0.54
1:L:15:LEU:HA	1:L:18:ALA:HB3	1.89	0.54
1:B:49:ALA:CB	1:B:115:LEU:HB3	2.38	0.54
1:H:196:ILE:HG22	1:H:197:ASN:H	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:2:THR:CG2	1:J:3:LEU:H	2.16	0.54
1:A:97:MET:HE2	1:A:158:HIS:HB2	1.88	0.54
1:C:252:MET:HE1	1:C:255:LYS:HD2	1.89	0.54
1:H:41:SER:O	1:H:43:GLU:N	2.41	0.54
1:H:58:VAL:O	1:H:58:VAL:HG12	2.08	0.54
1:K:46:ALA:O	1:K:49:ALA:HB3	2.07	0.54
1:G:184:PRO:HG3	1:G:198:ALA:HB2	1.89	0.54
1:B:154:ILE:CG2	1:B:155:ASP:N	2.69	0.54
1:D:223:LEU:C	1:D:223:LEU:HD23	2.27	0.54
1:G:55:MET:HG2	1:G:285:ILE:HD12	1.89	0.54
1:H:295:ILE:CG2	1:H:296:SER:N	2.70	0.54
1:G:15:LEU:CB	1:I:54:LEU:HD21	2.37	0.54
1:A:66:HIS:O	1:A:184:PRO:HD3	2.08	0.54
1:A:242:LEU:HD12	1:A:247:THR:HB	1.90	0.54
1:B:104:LEU:O	1:B:109:ASN:HB2	2.08	0.54
1:C:33:LYS:HA	1:C:65:VAL:O	2.08	0.54
1:D:51:ASP:OD1	1:D:279:ASN:ND2	2.40	0.54
1:F:101:GLU:HG3	1:F:185:ILE:HD13	1.90	0.54
1:G:39:MET:CE	1:G:44:LEU:CD2	2.84	0.54
1:G:11:VAL:HG12	1:I:286:PHE:CE2	2.43	0.54
1:K:213:LYS:NZ	1:K:271:HIS:CE1	2.75	0.54
1:L:220:ILE:HG21	3:L:1300:ADP:C2	2.43	0.54
1:L:237:GLU:HA	1:L:240:ASN:ND2	2.22	0.54
1:L:30:LEU:HD11	1:L:285:ILE:HD11	1.88	0.54
1:L:84:HIS:O	1:L:91:VAL:HG23	2.08	0.54
1:A:30:LEU:HD13	1:A:55:MET:HE3	1.89	0.54
1:B:218:THR:HG23	1:B:219:ASN:N	2.23	0.54
1:E:235:SER:N	1:E:238:GLN:HE21	1.98	0.54
1:F:243:ILE:O	1:F:246:GLY:HA2	2.08	0.54
1:G:8:ALA:CB	1:I:287:THR:CG2	2.86	0.54
1:K:109:ASN:HD21	1:K:125:GLY:CA	2.19	0.54
1:C:200:LEU:HD23	1:C:258:CYS:SG	2.48	0.54
1:C:215:MET:CE	1:C:284:GLU:HB2	2.38	0.54
1:F:243:ILE:HD12	1:F:248:ILE:HD13	1.90	0.54
1:G:8:ALA:CB	1:I:287:THR:HG21	2.36	0.54
1:I:215:MET:HE3	1:I:281:VAL:HG13	1.90	0.54
1:J:134:ILE:HD13	1:J:201:VAL:HG11	1.89	0.54
1:J:25:PHE:CD2	1:J:212:GLU:HG2	2.43	0.54
1:J:30:LEU:HD22	1:J:215:MET:HE2	1.89	0.54
1:J:86:ILE:HG22	1:J:89:MET:O	2.08	0.54
1:K:227:GLN:O	1:K:228:GLY:C	2.46	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:296:SER:O	1:K:297:ASN:CB	2.54	0.54
1:K:82:GLU:OE2	1:K:82:GLU:HA	2.07	0.54
1:L:162:VAL:HG11	1:L:204:LYS:HB3	1.90	0.54
1:L:30:LEU:HD22	1:L:213:LYS:HB3	1.89	0.54
1:B:97:MET:CE	1:B:195:ASN:N	2.71	0.54
1:B:50:ARG:NH2	1:C:12:ALA:HB1	2.22	0.54
1:F:93:ASP:OD1	1:F:96:THR:HG23	2.08	0.54
1:H:5:ARG:HG3	1:H:6:ASP:N	2.22	0.54
1:L:50:ARG:HG2	1:L:119:HIS:ND1	2.23	0.54
1:A:36:GLY:O	1:A:38:ALA:N	2.41	0.53
1:B:68:GLY:HA3	1:B:104:LEU:HD21	1.90	0.53
1:C:86:ILE:HG13	1:C:91:VAL:CG2	2.38	0.53
1:I:87:ASP:OD1	1:I:253:LEU:HD13	2.08	0.53
1:I:69:GLY:O	1:I:72:ILE:HB	2.08	0.53
1:J:7:ASP:O	1:J:10:GLN:HB2	2.08	0.53
1:H:23:ARG:NH2	1:L:120:GLY:O	2.41	0.53
1:A:36:GLY:CA	1:A:39:MET:HG2	2.38	0.53
1:G:101:GLU:HA	1:G:185:ILE:HD13	1.88	0.53
1:H:25:PHE:HB2	1:H:60:ILE:CD1	2.39	0.53
1:I:53:VAL:O	1:I:56:LYS:HB3	2.08	0.53
1:B:54:LEU:HD21	1:C:15:LEU:CD2	2.28	0.53
1:B:58:VAL:O	1:B:58:VAL:CG1	2.57	0.53
1:B:68:GLY:O	1:B:70:PRO:CD	2.57	0.53
1:F:207:GLU:CD	1:F:265:GLY:HA3	2.29	0.53
1:H:220:ILE:O	1:H:222:GLY:N	2.41	0.53
1:H:248:ILE:HG23	1:H:252:MET:HB2	1.90	0.53
1:H:253:LEU:HB3	1:H:254:PRO:CD	2.37	0.53
1:A:257:ARG:O	1:A:261:GLU:HG3	2.07	0.53
1:B:252:MET:CE	1:B:255:LYS:HD2	2.38	0.53
1:D:128:GLY:HA3	1:D:185:ILE:O	2.08	0.53
1:H:19:LEU:CD2	1:L:53:VAL:HG11	2.38	0.53
1:J:134:ILE:HD13	1:J:201:VAL:CG1	2.37	0.53
1:K:285:ILE:HG13	1:K:286:PHE:N	2.24	0.53
1:G:255:LYS:HE3	3:G:1299:ADP:O2B	2.08	0.53
1:J:253:LEU:CB	1:J:254:PRO:HD3	2.30	0.53
1:C:24:ARG:HD3	1:C:25:PHE:CE2	2.43	0.53
1:H:249:TYR:HD1	1:H:249:TYR:O	1.91	0.53
1:I:117:ASN:ND2	1:I:123:ALA:CB	2.70	0.53
1:I:141:VAL:HG21	1:I:156:ILE:CD1	2.39	0.53
1:J:212:GLU:O	1:J:268:THR:HB	2.09	0.53
1:J:69:GLY:N	1:J:70:PRO:CD	2.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:279:ASN:O	1:K:283:LEU:HG	2.09	0.53
1:F:235:SER:O	1:F:238:GLN:HB3	2.09	0.53
1:G:148:MET:HE1	1:G:152:GLU:HB3	1.89	0.53
1:J:22:ILE:HG23	1:J:58:VAL:HG13	1.91	0.53
1:L:242:LEU:HB2	1:L:248:ILE:HD12	1.91	0.53
1:B:252:MET:HE1	1:B:255:LYS:HD2	1.89	0.53
1:H:207:GLU:HG3	1:H:262:ALA:HA	1.91	0.53
1:J:54:LEU:O	1:J:58:VAL:CG2	2.55	0.53
1:D:143:ARG:HB2	1:D:154:ILE:HD12	1.89	0.53
1:H:46:ALA:HA	1:H:115:LEU:HD21	1.91	0.53
1:L:232:THR:CG2	1:L:294:LEU:H	2.21	0.53
1:C:74:ASP:O	1:C:78:ARG:HG3	2.09	0.52
1:E:219:ASN:O	1:E:276:ARG:NE	2.42	0.52
1:E:66:HIS:NE2	1:E:109:ASN:HB2	2.24	0.52
1:A:101:GLU:HG2	1:A:185:ILE:HD13	1.90	0.52
1:D:213:LYS:NZ	1:D:271:HIS:CE1	2.76	0.52
1:H:223:LEU:CD1	1:H:248:ILE:HG12	2.39	0.52
1:I:141:VAL:HG12	1:I:142:THR:N	2.22	0.52
1:K:49:ALA:O	1:K:53:VAL:HG23	2.09	0.52
1:L:223:LEU:HD13	1:L:256:ILE:CD1	2.38	0.52
1:A:10:GLN:HE22	1:E:10:GLN:HG3	1.72	0.52
1:D:254:PRO:O	1:D:258:CYS:HB3	2.09	0.52
1:F:133:LEU:HG	1:F:134:ILE:HG12	1.90	0.52
1:F:253:LEU:HB3	1:F:254:PRO:HD3	1.92	0.52
1:G:287:THR:HG22	1:G:288:ASP:N	2.24	0.52
1:H:175:LYS:HG2	1:H:175:LYS:O	2.07	0.52
1:J:161:GLU:HA	1:J:196:ILE:HD13	1.91	0.52
1:A:10:GLN:O	1:A:14:VAL:HG23	2.09	0.52
1:B:178:PHE:O	1:B:180:PRO:HD3	2.09	0.52
1:D:195:ASN:ND2	2:D:1302:NLG:H8C1	2.24	0.52
1:F:74:ASP:O	1:F:78:ARG:HG3	2.10	0.52
1:I:133:LEU:HD12	1:I:133:LEU:O	2.10	0.52
1:I:224:MET:HE2	1:I:228:GLY:HA2	1.91	0.52
1:J:219:ASN:HD21	1:J:220:ILE:HG13	1.69	0.52
1:L:90:ARG:H	2:L:1302:NLG:H8C2	1.74	0.52
1:F:243:ILE:HG22	1:F:244:ALA:N	2.25	0.52
1:B:57:ALA:HB2	1:C:19:LEU:HD21	1.90	0.52
1:H:101:GLU:HA	1:H:185:ILE:CD1	2.39	0.52
1:L:30:LEU:HD13	1:L:215:MET:HE1	1.91	0.52
1:F:261:GLU:O	1:F:265:GLY:N	2.41	0.52
1:I:93:ASP:OD2	1:I:96:THR:HG23	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:225:ASP:OD1	1:J:225:ASP:C	2.48	0.52
1:K:131:ALA:N	1:L:123:ALA:O	2.40	0.52
1:A:245:ASP:C	1:A:245:ASP:OD1	2.47	0.52
1:B:128:GLY:CA	1:B:185:ILE:O	2.57	0.52
1:C:271:HIS:CE1	1:C:294:LEU:HD13	2.44	0.52
1:F:35:GLY:HA3	1:F:67:GLY:H	1.75	0.52
1:H:30:LEU:HD11	1:H:215:MET:SD	2.49	0.52
1:H:90:ARG:HG2	1:H:91:VAL:N	2.23	0.52
1:J:296:SER:C	1:J:298:ARG:N	2.62	0.52
1:K:92:THR:HG21	1:K:97:MET:HE3	1.90	0.52
1:E:30:LEU:HD11	1:E:213:LYS:HG2	1.92	0.52
1:G:39:MET:O	1:G:39:MET:HG3	2.10	0.52
1:H:63:VAL:HG22	1:H:180:PRO:HG2	1.92	0.52
1:H:22:ILE:CD1	1:H:286:PHE:HE2	2.22	0.52
1:I:263:VAL:HG11	1:I:296:SER:O	2.10	0.52
1:K:271:HIS:NE2	1:K:294:LEU:CD1	2.73	0.52
1:A:52:VAL:HG12	1:A:179:ILE:HD13	1.92	0.52
1:B:131:ALA:HB3	1:B:169:LEU:HD22	1.92	0.52
1:B:260:LEU:O	1:B:264:GLN:HG2	2.10	0.52
1:G:223:LEU:HD11	1:G:248:ILE:HG12	1.91	0.52
1:I:92:THR:HG22	1:I:96:THR:HG1	1.75	0.52
1:J:218:THR:HG22	1:J:273:ILE:O	2.09	0.52
1:A:224:MET:HB3	1:A:229:GLN:O	2.10	0.51
1:D:89:MET:HE2	1:D:159:VAL:HG11	1.90	0.51
1:F:3:LEU:CD2	1:F:8:ALA:HA	2.41	0.51
1:G:104:LEU:O	1:G:109:ASN:HB2	2.09	0.51
1:G:226:LYS:C	1:G:228:GLY:N	2.61	0.51
1:H:141:VAL:CG2	1:H:156:ILE:HD12	2.29	0.51
1:I:184:PRO:HG2	1:I:198:ALA:HB2	1.92	0.51
1:K:30:LEU:HD23	1:K:213:LYS:HB2	1.92	0.51
1:L:197:ASN:HB3	1:L:200:LEU:HD12	1.92	0.51
1:L:237:GLU:CD	1:L:237:GLU:H	2.13	0.51
1:B:101:GLU:HA	1:B:185:ILE:HD11	1.88	0.51
1:B:141:VAL:HG21	1:B:156:ILE:HD11	1.92	0.51
1:D:219:ASN:ND2	1:D:219:ASN:C	2.56	0.51
1:D:3:LEU:HD12	1:F:287:THR:CG2	2.39	0.51
1:F:97:MET:HE3	1:F:195:ASN:HB2	1.92	0.51
1:H:18:ALA:O	1:H:22:ILE:HD12	2.11	0.51
1:H:273:ILE:CG2	1:H:274:ASP:N	2.74	0.51
1:I:36:GLY:O	1:I:40:GLU:HG2	2.09	0.51
1:H:287:THR:HG21	1:L:3:LEU:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:LYS:HD3	1:A:187:VAL:HG13	1.92	0.51
1:B:271:HIS:ND1	1:B:284:GLU:OE2	2.43	0.51
1:E:139:LEU:H	1:E:160:GLY:HA2	1.76	0.51
1:E:33:LYS:HA	1:E:65:VAL:O	2.11	0.51
1:F:89:MET:CE	1:F:139:LEU:CD2	2.88	0.51
1:G:4:SER:OG	1:G:7:ASP:HB2	2.10	0.51
1:H:220:ILE:HG13	1:H:224:MET:CE	2.41	0.51
1:H:234:LEU:HD23	1:H:238:GLN:CB	2.38	0.51
1:I:72:ILE:HG23	1:I:76:LEU:HD12	1.89	0.51
1:K:34:TYR:CZ	1:K:45:LYS:HE3	2.45	0.51
1:J:19:LEU:HD22	1:K:54:LEU:HD12	1.92	0.51
1:L:219:ASN:O	1:L:276:ARG:CZ	2.59	0.51
1:A:101:GLU:HG3	1:A:185:ILE:HD13	1.92	0.51
1:C:232:THR:HG22	1:C:294:LEU:HB3	1.92	0.51
1:H:48:PHE:O	1:H:51:ASP:HB2	2.11	0.51
1:J:39:MET:HA	1:J:44:LEU:CD1	2.40	0.51
1:K:173:LEU:HD22	1:K:178:PHE:HB2	1.91	0.51
1:A:294:LEU:C	1:A:294:LEU:HD12	2.30	0.51
1:A:36:GLY:HA3	1:A:39:MET:SD	2.51	0.51
1:E:218:THR:HB	1:E:255:LYS:HE2	1.90	0.51
1:G:148:MET:HE3	1:G:152:GLU:HB3	1.90	0.51
1:I:178:PHE:HE1	1:J:172:MET:CE	2.23	0.51
1:J:123:ALA:O	1:J:124:ILE:HD12	2.10	0.51
1:J:252:MET:HE2	1:J:272:ILE:HD13	1.92	0.51
1:A:250:GLY:O	1:A:254:PRO:HD3	2.10	0.51
1:B:239:VAL:O	1:B:243:ILE:HG13	2.11	0.51
1:D:242:LEU:CD2	1:D:247:THR:HG21	2.38	0.51
1:E:287:THR:HG22	1:E:288:ASP:N	2.24	0.51
1:F:87:ASP:OD1	1:F:87:ASP:O	2.28	0.51
1:G:263:VAL:HA	1:G:267:VAL:O	2.11	0.51
1:J:232:THR:HG23	1:J:294:LEU:HB3	1.93	0.51
1:J:79:LEU:O	1:J:79:LEU:HG	2.10	0.51
1:K:224:MET:CB	1:K:229:GLN:H	2.23	0.51
1:L:84:HIS:CE1	1:L:91:VAL:HG21	2.42	0.51
1:E:10:GLN:CG	1:E:11:VAL:N	2.72	0.51
1:F:51:ASP:OD2	1:F:279:ASN:HA	2.10	0.51
1:I:195:ASN:C	1:I:196:ILE:HG13	2.30	0.51
1:J:66:HIS:O	1:J:184:PRO:CD	2.58	0.51
1:J:37:ASN:OD1	1:J:37:ASN:N	2.43	0.51
1:B:97:MET:HE1	1:B:194:TYR:CA	2.41	0.51
1:B:22:ILE:HG22	1:B:26:VAL:HG23	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:25:PHE:CE2	1:C:213:LYS:HE2	2.46	0.51
1:G:172:MET:O	1:H:172:MET:CE	2.58	0.51
1:I:99:VAL:O	1:I:102:MET:CG	2.58	0.51
1:I:107:GLN:HG2	1:I:108:VAL:N	2.25	0.51
1:I:257:ARG:O	1:I:261:GLU:HG3	2.11	0.51
1:I:81:ILE:CG2	1:I:82:GLU:H	2.24	0.51
1:K:124:ILE:HD11	1:L:169:LEU:CD1	2.35	0.51
1:A:223:LEU:HD21	1:A:248:ILE:HG12	1.92	0.51
1:B:259:ALA:O	1:B:263:VAL:HG23	2.10	0.51
1:E:262:ALA:HB1	1:E:267:VAL:HG21	1.91	0.51
1:J:221:ALA:CB	1:J:230:VAL:HG22	2.40	0.51
1:K:285:ILE:HG13	1:K:286:PHE:CD2	2.46	0.51
1:L:104:LEU:O	1:L:109:ASN:HB2	2.10	0.51
1:A:36:GLY:HA3	1:A:39:MET:HG2	1.93	0.51
1:B:144:GLN:CD	1:B:149:THR:HG21	2.30	0.51
1:B:50:ARG:NH2	1:B:279:ASN:HD21	2.09	0.51
1:E:221:ALA:HB2	1:E:274:ASP:HB2	1.93	0.51
1:H:18:ALA:C	1:H:22:ILE:HD12	2.31	0.51
1:I:10:GLN:O	1:I:14:VAL:HG23	2.11	0.51
1:L:22:ILE:CD1	1:L:58:VAL:HG11	2.41	0.51
1:B:212:GLU:OE1	1:B:212:GLU:HA	2.09	0.50
1:B:30:LEU:CD2	1:B:55:MET:SD	2.99	0.50
1:E:170:LEU:HD13	1:E:209:LEU:HD11	1.92	0.50
1:E:93:ASP:OD1	1:E:96:THR:OG1	2.29	0.50
1:G:25:PHE:HB2	1:G:60:ILE:HD13	1.93	0.50
1:I:79:LEU:HD13	1:J:78:ARG:CG	2.38	0.50
1:J:157:GLY:O	1:J:159:VAL:N	2.44	0.50
1:K:103:VAL:HA	1:K:107:GLN:HG2	1.93	0.50
1:K:170:LEU:O	1:K:174:VAL:HG23	2.10	0.50
1:L:40:GLU:O	1:L:40:GLU:HG3	2.11	0.50
1:B:46:ALA:HA	1:B:115:LEU:HG	1.93	0.50
1:F:23:ARG:HA	1:F:26:VAL:HG23	1.93	0.50
1:I:101:GLU:HA	1:I:185:ILE:HD13	1.90	0.50
1:L:54:LEU:O	1:L:58:VAL:HG23	2.11	0.50
1:L:58:VAL:HG12	1:L:58:VAL:O	2.12	0.50
1:B:50:ARG:HB2	1:B:119:HIS:HD2	1.77	0.50
1:E:251:GLY:O	1:E:254:PRO:HD2	2.11	0.50
1:E:55:MET:SD	1:E:281:VAL:HG11	2.51	0.50
1:F:85:PHE:CB	1:F:90:ARG:HA	2.40	0.50
1:G:235:SER:O	1:G:239:VAL:HG23	2.10	0.50
1:K:257:ARG:O	1:K:261:GLU:HG3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:99:VAL:HG12	1:K:100:VAL:N	2.26	0.50
1:D:35:GLY:C	1:D:37:ASN:H	2.14	0.50
1:D:3:LEU:CD2	1:D:3:LEU:N	2.67	0.50
1:G:84:HIS:HA	1:G:85:PHE:CD1	2.45	0.50
1:J:223:LEU:CD1	1:J:248:ILE:HD13	2.41	0.50
1:B:143:ARG:HG2	1:B:154:ILE:HG13	1.93	0.50
1:C:5:ARG:HH11	1:C:5:ARG:CG	2.24	0.50
1:F:11:VAL:HG13	1:F:15:LEU:CG	2.40	0.50
1:F:235:SER:O	1:F:239:VAL:HG23	2.11	0.50
1:G:142:THR:HG22	1:G:143:ARG:HD2	1.94	0.50
1:H:220:ILE:HG21	3:H:1297:ADP:C3'	2.42	0.50
1:J:223:LEU:CD1	1:J:248:ILE:HD11	2.38	0.50
1:C:248:ILE:CG2	1:C:256:ILE:HD11	2.42	0.50
1:C:253:LEU:CD2	1:C:257:ARG:NH1	2.74	0.50
1:F:219:ASN:ND2	1:F:219:ASN:C	2.65	0.50
1:G:212:GLU:O	1:G:268:THR:HB	2.11	0.50
1:H:25:PHE:O	1:H:60:ILE:HG12	2.12	0.50
1:I:117:ASN:HD21	1:I:123:ALA:CA	2.25	0.50
1:J:220:ILE:HD11	3:J:1298:ADP:O3'	2.09	0.50
1:J:72:ILE:HG21	1:J:90:ARG:HH22	1.75	0.50
1:A:117:ASN:ND2	1:A:121:GLY:O	2.45	0.50
1:A:24:ARG:NH2	1:A:288:ASP:HB2	2.26	0.50
1:C:32:ILE:HD13	1:C:281:VAL:HG21	1.92	0.50
1:F:22:ILE:HG21	1:F:58:VAL:CG1	2.42	0.50
1:F:58:VAL:O	1:F:58:VAL:CG1	2.59	0.50
1:C:90:ARG:NH1	1:I:227:GLN:O	2.45	0.50
1:I:294:LEU:HD12	1:I:295:ILE:N	2.27	0.50
1:K:270:ALA:O	1:K:295:ILE:HG22	2.11	0.50
1:F:51:ASP:O	1:F:55:MET:HG3	2.12	0.50
1:G:142:THR:CG2	1:G:143:ARG:HD2	2.42	0.50
1:G:46:ALA:HB1	1:G:119:HIS:HE1	1.76	0.50
1:H:101:GLU:HA	1:H:185:ILE:HD11	1.94	0.50
1:I:209:LEU:O	1:I:210:LYS:C	2.49	0.50
1:K:75:LEU:CD2	1:L:102:MET:SD	3.00	0.50
1:A:7:ASP:O	1:A:10:GLN:HB3	2.12	0.50
1:A:93:ASP:OD2	1:A:96:THR:CG2	2.59	0.50
1:B:85:PHE:N	1:B:85:PHE:CD1	2.80	0.50
1:F:75:LEU:O	1:F:76:LEU:C	2.49	0.50
1:H:188:GLY:HA3	1:H:192:GLU:OE2	2.12	0.50
1:H:209:LEU:O	1:H:210:LYS:HB2	2.11	0.50
1:H:268:THR:O	1:H:269:SER:HB3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:143:ARG:CB	1:I:154:ILE:HG13	2.42	0.50
1:K:107:GLN:HG3	1:K:108:VAL:H	1.77	0.50
1:K:129:LYS:NZ	1:K:187:VAL:CG1	2.68	0.50
1:A:232:THR:HG21	1:A:290:GLY:O	2.11	0.49
1:A:245:ASP:OD1	1:A:246:GLY:N	2.45	0.49
1:D:225:ASP:HB3	1:D:227:GLN:H	1.75	0.49
1:D:239:VAL:O	1:D:243:ILE:HG22	2.12	0.49
1:E:218:THR:HG22	1:E:273:ILE:O	2.11	0.49
1:I:156:ILE:HG22	1:I:159:VAL:HB	1.94	0.49
1:L:252:MET:CE	1:L:255:LYS:HD2	2.42	0.49
1:B:19:LEU:HD21	1:C:53:VAL:CG1	2.42	0.49
1:B:34:TYR:HE2	1:B:39:MET:HG3	1.77	0.49
1:G:138:LYS:NZ	1:G:155:ASP:HA	2.27	0.49
1:G:223:LEU:HD23	1:G:234:LEU:CD1	2.42	0.49
1:G:248:ILE:HD13	1:G:256:ILE:HD13	1.94	0.49
1:H:290:GLY:HA2	1:H:294:LEU:HD13	1.94	0.49
1:H:97:MET:HE2	1:H:97:MET:CA	2.31	0.49
1:K:213:LYS:HD2	1:K:269:SER:OG	2.12	0.49
1:K:81:ILE:HG22	1:K:82:GLU:N	2.26	0.49
1:L:55:MET:O	1:L:60:ILE:N	2.43	0.49
1:A:39:MET:HA	1:A:44:LEU:HD12	1.94	0.49
1:A:35:GLY:HA2	1:A:40:GLU:OE1	2.12	0.49
1:A:30:LEU:HD12	1:A:55:MET:HE2	1.94	0.49
1:A:80:SER:OG	1:A:80:SER:O	2.30	0.49
1:B:15:LEU:HD11	1:C:15:LEU:CD1	2.43	0.49
1:C:58:VAL:CG1	1:C:58:VAL:O	2.60	0.49
1:D:282:LEU:HD11	1:D:286:PHE:CD2	2.48	0.49
1:D:54:LEU:HD13	1:D:282:LEU:HD13	1.94	0.49
1:E:129:LYS:HE3	1:F:114:ASN:HB2	1.94	0.49
1:F:16:SER:HA	1:F:19:LEU:HD12	1.93	0.49
1:H:19:LEU:O	1:H:23:ARG:HG3	2.11	0.49
1:I:154:ILE:O	1:I:154:ILE:HG22	2.13	0.49
1:J:55:MET:O	1:J:60:ILE:HB	2.12	0.49
1:K:216:LEU:HB2	1:K:272:ILE:HG12	1.93	0.49
1:K:76:LEU:HD21	1:K:99:VAL:HG11	1.94	0.49
1:A:235:SER:OG	1:A:238:GLN:NE2	2.45	0.49
1:B:143:ARG:O	1:B:144:GLN:HG3	2.13	0.49
1:B:149:THR:HG22	1:B:150:LYS:H	1.74	0.49
1:B:134:ILE:CD1	1:B:201:VAL:HG13	2.42	0.49
1:E:167:VAL:CG1	1:E:209:LEU:HD23	2.33	0.49
1:F:157:GLY:O	1:F:159:VAL:HG23	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:253:LEU:HB3	1:F:254:PRO:CD	2.42	0.49
1:G:3:LEU:HD12	1:G:4:SER:H	1.76	0.49
1:H:44:LEU:HD23	1:H:275:GLY:O	2.13	0.49
1:G:11:VAL:HG22	1:I:15:LEU:HD23	1.93	0.49
1:I:23:ARG:NH1	1:I:23:ARG:HG2	2.28	0.49
1:J:30:LEU:HD22	1:J:213:LYS:HB2	1.90	0.49
1:K:203:GLY:HA2	1:K:214:LEU:HD21	1.94	0.49
1:L:197:ASN:ND2	2:L:1302:NLG:OE1	2.45	0.49
1:A:285:ILE:HG22	1:A:286:PHE:N	2.27	0.49
1:B:37:ASN:HB2	1:B:219:ASN:CG	2.31	0.49
1:E:79:LEU:O	1:E:80:SER:HB2	2.12	0.49
1:B:141:VAL:HG21	1:B:156:ILE:CD1	2.42	0.49
1:C:249:TYR:O	3:C:1300:ADP:C8	2.66	0.49
1:D:55:MET:O	1:D:60:ILE:HB	2.12	0.49
1:F:19:LEU:HB2	1:F:20:PRO:HD3	1.95	0.49
1:F:243:ILE:CG2	1:F:244:ALA:N	2.75	0.49
1:G:248:ILE:HD13	1:G:256:ILE:HD12	1.93	0.49
1:H:172:MET:O	1:H:175:LYS:NZ	2.41	0.49
1:I:75:LEU:HD22	1:I:103:VAL:CG2	2.41	0.49
1:J:25:PHE:CE2	1:J:213:LYS:HE3	2.48	0.49
1:K:229:GLN:O	1:K:231:LEU:HD12	2.11	0.49
1:L:55:MET:SD	1:L:60:ILE:HD13	2.52	0.49
1:A:58:VAL:HG12	1:A:58:VAL:O	2.12	0.49
1:C:44:LEU:CD2	1:C:276:ARG:HA	2.43	0.49
1:F:271:HIS:CE1	1:F:284:GLU:HG3	2.46	0.49
1:H:8:ALA:HB3	1:L:279:ASN:HD21	1.78	0.49
1:I:110:LYS:NZ	1:J:130:ASP:OD2	2.45	0.49
1:J:3:LEU:HD22	1:K:21:TYR:CZ	2.48	0.49
1:L:52:VAL:CG1	1:L:179:ILE:HD13	2.43	0.49
1:A:192:GLU:OE2	1:A:194:TYR:CE1	2.66	0.49
1:B:149:THR:CG2	1:B:150:LYS:H	2.26	0.49
1:D:188:GLY:HA3	1:D:192:GLU:OE2	2.12	0.49
1:E:30:LEU:HD23	1:E:55:MET:HE1	1.93	0.49
1:G:72:ILE:HD12	1:G:90:ARG:NH2	2.25	0.49
1:H:239:VAL:HG11	1:H:260:LEU:HD11	1.95	0.49
1:J:23:ARG:HA	1:J:26:VAL:HG23	1.94	0.49
1:C:19:LEU:N	1:C:20:PRO:CD	2.76	0.49
1:C:222:GLY:HA3	1:C:230:VAL:HG13	1.95	0.49
1:E:33:LYS:HE2	1:E:198:ALA:HB3	1.94	0.49
1:G:143:ARG:HG3	1:G:144:GLN:H	1.77	0.49
1:G:195:ASN:C	1:G:196:ILE:HG13	2.32	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:22:ILE:CD1	1:H:286:PHE:CE2	2.94	0.49
1:H:50:ARG:O	1:H:54:LEU:HB2	2.13	0.49
1:K:66:HIS:CE1	1:K:183:ALA:HA	2.47	0.49
1:L:223:LEU:HD11	1:L:248:ILE:HD11	1.94	0.49
1:A:223:LEU:HD12	1:A:224:MET:N	2.28	0.49
1:B:11:VAL:CG2	1:C:14:VAL:HG12	2.42	0.49
1:C:35:GLY:HA3	1:C:67:GLY:H	1.78	0.49
1:I:66:HIS:O	1:I:184:PRO:HD3	2.13	0.49
1:I:223:LEU:HD23	1:I:256:ILE:CD1	2.41	0.49
1:I:257:ARG:O	1:I:261:GLU:HG2	2.13	0.49
1:J:216:LEU:HD12	1:J:255:LYS:HG2	1.94	0.49
1:K:172:MET:CE	1:L:172:MET:HG3	2.42	0.49
1:K:213:LYS:NZ	1:K:271:HIS:HE1	2.10	0.49
1:A:273:ILE:HG22	1:A:274:ASP:N	2.27	0.48
1:B:184:PRO:HG3	1:B:198:ALA:HB2	1.95	0.48
1:H:227:GLN:HG3	1:H:228:GLY:N	2.27	0.48
1:I:238:GLN:O	1:I:241:GLU:HB2	2.13	0.48
1:I:42:GLU:O	1:I:45:LYS:HB3	2.13	0.48
1:K:26:VAL:HG13	1:K:59:GLY:HA3	1.95	0.48
1:L:139:LEU:HD12	1:L:140:THR:N	2.28	0.48
1:A:295:ILE:O	1:A:296:SER:HB3	2.13	0.48
1:D:2:THR:N	1:F:21:TYR:HH	2.11	0.48
1:K:5:ARG:CG	1:K:6:ASP:N	2.56	0.48
1:A:58:VAL:CG1	1:A:58:VAL:O	2.60	0.48
1:B:23:ARG:HD3	1:C:120:GLY:HA3	1.96	0.48
1:E:256:ILE:O	1:E:259:ALA:N	2.46	0.48
1:F:259:ALA:O	1:F:260:LEU:C	2.52	0.48
1:F:291:VAL:O	1:F:291:VAL:HG12	2.13	0.48
1:F:65:VAL:HG21	1:F:202:ALA:HA	1.95	0.48
1:I:86:ILE:HD13	1:I:154:ILE:HD13	1.95	0.48
1:J:230:VAL:CG1	1:J:292:GLY:HA2	2.41	0.48
1:J:288:ASP:O	1:J:290:GLY:N	2.46	0.48
1:K:44:LEU:HA	1:K:44:LEU:HD12	1.58	0.48
1:L:46:ALA:O	1:L:50:ARG:HG3	2.13	0.48
1:A:39:MET:H	1:A:39:MET:CE	2.25	0.48
1:B:50:ARG:CB	1:B:119:HIS:HD2	2.27	0.48
1:D:137:LYS:HE3	1:D:161:GLU:OE1	2.14	0.48
1:F:52:VAL:HG12	1:F:179:ILE:HD13	1.95	0.48
1:G:143:ARG:CZ	1:G:151:PRO:CG	2.91	0.48
1:I:46:ALA:O	1:I:50:ARG:HG3	2.13	0.48
1:J:217:LEU:CD2	1:J:273:ILE:HB	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:253:LEU:N	1:L:254:PRO:CD	2.76	0.48
1:E:211:ALA:O	1:E:267:VAL:HG13	2.13	0.48
1:A:3:LEU:HD13	1:E:286:PHE:O	2.13	0.48
1:F:73:GLY:HA2	1:F:76:LEU:HD12	1.95	0.48
1:H:196:ILE:CG2	1:H:197:ASN:N	2.77	0.48
1:H:262:ALA:O	1:H:265:GLY:N	2.46	0.48
1:J:19:LEU:HA	1:J:22:ILE:CD1	2.41	0.48
1:K:178:PHE:HE1	1:L:172:MET:SD	2.37	0.48
1:L:287:THR:CG2	1:L:288:ASP:N	2.76	0.48
1:A:256:ILE:HD12	1:A:272:ILE:CD1	2.43	0.48
1:C:245:ASP:OD1	1:C:247:THR:HG23	2.14	0.48
1:C:248:ILE:HG21	1:C:256:ILE:CD1	2.44	0.48
1:E:35:GLY:CA	1:E:39:MET:CG	2.82	0.48
1:F:133:LEU:CD2	1:F:182:ILE:CG2	2.91	0.48
1:G:75:LEU:CG	1:G:79:LEU:HD11	2.36	0.48
1:H:32:ILE:HD13	1:H:281:VAL:HG11	1.95	0.48
1:G:9:ALA:HA	1:I:283:LEU:CD2	2.41	0.48
1:K:66:HIS:O	1:K:184:PRO:CD	2.61	0.48
1:C:5:ARG:HH11	1:C:5:ARG:HG3	1.79	0.48
1:G:273:ILE:CG2	1:G:274:ASP:N	2.76	0.48
1:H:35:GLY:CA	1:H:67:GLY:H	2.21	0.48
1:I:7:ASP:O	1:I:11:VAL:CG2	2.58	0.48
1:J:13:LYS:O	1:J:17:GLU:HG3	2.12	0.48
1:J:25:PHE:O	1:J:27:GLY:N	2.47	0.48
1:K:203:GLY:HA2	1:K:214:LEU:CD2	2.44	0.48
1:C:28:LYS:CG	1:C:29:THR:N	2.65	0.48
1:E:75:LEU:O	1:E:79:LEU:HD12	2.13	0.48
1:F:237:GLU:O	1:F:241:GLU:HG3	2.14	0.48
1:I:103:VAL:HG12	1:I:104:LEU:HD23	1.96	0.48
1:J:38:ALA:C	1:J:40:GLU:N	2.67	0.48
1:J:39:MET:HA	1:J:44:LEU:HD12	1.95	0.48
1:K:25:PHE:C	1:K:27:GLY:H	2.15	0.48
1:C:215:MET:HE1	1:C:284:GLU:HB2	1.95	0.48
1:C:277:VAL:O	1:C:280:ALA:HB2	2.14	0.48
1:E:251:GLY:HA3	3:E:1299:ADP:PA	2.54	0.48
1:H:229:GLN:HG2	1:H:231:LEU:HD23	1.96	0.48
1:H:75:LEU:HD23	1:H:99:VAL:HG13	1.96	0.48
1:A:253:LEU:HB3	1:A:254:PRO:HD3	1.96	0.48
1:C:135:ARG:HH21	1:C:164:GLY:HA3	1.79	0.48
1:C:127:THR:HG22	1:C:183:ALA:HB3	1.95	0.48
1:F:200:LEU:HA	1:F:258:CYS:SG	2.53	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:58:VAL:HG12	1:G:60:ILE:HG13	1.96	0.48
1:H:19:LEU:HG	1:H:23:ARG:CZ	2.44	0.48
1:I:115:LEU:O	1:I:118:ARG:HB2	2.14	0.48
1:I:173:LEU:O	1:I:178:PHE:HB2	2.14	0.48
1:I:213:LYS:HA	1:I:269:SER:O	2.14	0.48
1:I:58:VAL:CG1	1:I:58:VAL:O	2.61	0.48
1:I:29:THR:HG22	1:I:61:ASN:CB	2.41	0.48
1:J:285:ILE:HG23	1:J:286:PHE:CD1	2.48	0.48
1:L:30:LEU:HD12	1:L:55:MET:CE	2.44	0.48
1:C:248:ILE:HD13	1:C:256:ILE:HD13	1.94	0.47
1:D:143:ARG:O	1:D:151:PRO:HA	2.14	0.47
1:H:101:GLU:OE2	1:H:129:LYS:HD2	2.14	0.47
1:J:263:VAL:HG13	1:J:268:THR:O	2.14	0.47
1:L:72:ILE:HD11	1:L:104:LEU:HG	1.94	0.47
1:A:72:ILE:HD11	1:A:104:LEU:HG	1.96	0.47
1:F:22:ILE:CG2	1:F:58:VAL:CG1	2.92	0.47
1:G:11:VAL:HG23	1:I:14:VAL:CG1	2.44	0.47
1:H:222:GLY:O	3:H:1297:ADP:H2	1.97	0.47
1:H:240:ASN:HA	1:H:243:ILE:CG1	2.43	0.47
1:I:262:ALA:O	1:I:267:VAL:CB	2.62	0.47
1:J:220:ILE:HD11	3:J:1298:ADP:C2'	2.44	0.47
1:J:7:ASP:HA	1:J:10:GLN:HB2	1.96	0.47
1:L:101:GLU:HA	1:L:185:ILE:HD11	1.95	0.47
1:C:271:HIS:ND1	1:C:284:GLU:OE1	2.47	0.47
1:H:199:ASP:CG	1:H:216:LEU:HD21	2.33	0.47
1:L:42:GLU:HA	1:L:45:LYS:HD3	1.95	0.47
1:C:18:ALA:HA	1:C:21:TYR:HD1	1.79	0.47
1:D:239:VAL:O	1:D:243:ILE:CG2	2.62	0.47
1:E:30:LEU:HD23	1:E:55:MET:CE	2.44	0.47
1:E:76:LEU:HD12	1:E:81:ILE:HD13	1.94	0.47
1:K:104:LEU:HB2	1:K:185:ILE:HD11	1.96	0.47
1:A:263:VAL:HA	1:A:267:VAL:O	2.14	0.47
1:G:214:LEU:HD21	1:G:258:CYS:SG	2.53	0.47
1:I:66:HIS:O	1:I:184:PRO:CG	2.61	0.47
1:I:39:MET:HB2	1:I:44:LEU:CD2	2.44	0.47
1:J:19:LEU:N	1:J:20:PRO:CD	2.78	0.47
1:J:232:THR:CG2	1:J:294:LEU:HB3	2.44	0.47
1:J:73:GLY:O	1:J:77:LYS:HG3	2.14	0.47
1:K:72:ILE:CG1	1:K:103:VAL:HB	2.41	0.47
1:L:49:ALA:CB	1:L:115:LEU:HG	2.44	0.47
1:L:285:ILE:HG22	1:L:286:PHE:N	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:19:LEU:HD13	1:C:54:LEU:HD13	1.96	0.47
1:H:37:ASN:ND2	1:H:37:ASN:N	2.62	0.47
1:J:113:VAL:HG13	1:J:123:ALA:CB	2.44	0.47
1:I:178:PHE:CE1	1:J:172:MET:CE	2.97	0.47
1:J:263:VAL:HA	1:J:267:VAL:O	2.15	0.47
1:L:150:LYS:HB3	1:L:151:PRO:CD	2.45	0.47
1:C:248:ILE:HG21	1:C:256:ILE:HD11	1.97	0.47
1:H:218:THR:CG2	1:H:220:ILE:O	2.63	0.47
1:H:44:LEU:O	1:H:44:LEU:HG	2.14	0.47
1:I:74:ASP:O	1:I:78:ARG:HD3	2.14	0.47
1:J:118:ARG:NH1	1:J:118:ARG:HG3	2.30	0.47
1:J:223:LEU:HD13	1:J:248:ILE:HD13	1.96	0.47
1:J:224:MET:HA	1:J:229:GLN:O	2.14	0.47
1:L:19:LEU:O	1:L:22:ILE:N	2.48	0.47
1:A:273:ILE:HD11	1:A:284:GLU:CG	2.45	0.47
1:A:90:ARG:HG2	1:A:91:VAL:O	2.14	0.47
1:C:69:GLY:HA2	1:C:71:GLN:HE22	1.79	0.47
1:E:167:VAL:CG1	1:E:171:ASN:HD21	2.26	0.47
1:E:162:VAL:HG11	1:E:204:LYS:HB3	1.97	0.47
1:F:139:LEU:CD1	1:F:161:GLU:HG3	2.45	0.47
1:G:236:THR:O	1:G:240:ASN:ND2	2.47	0.47
1:I:102:MET:CE	1:J:75:LEU:HD22	2.44	0.47
1:I:124:ILE:CD1	1:I:173:LEU:HD22	2.42	0.47
1:K:97:MET:HE2	1:K:195:ASN:HB2	1.97	0.47
1:K:229:GLN:HB3	1:K:231:LEU:HD12	1.97	0.47
1:A:242:LEU:CD1	1:A:247:THR:HB	2.45	0.47
1:B:237:GLU:O	1:B:241:GLU:HG3	2.15	0.47
1:B:34:TYR:CD1	1:B:48:PHE:CE1	3.02	0.47
1:E:184:PRO:HB3	1:E:198:ALA:HA	1.96	0.47
1:H:44:LEU:CD2	1:H:275:GLY:O	2.63	0.47
1:B:109:ASN:HD21	1:B:125:GLY:CA	2.28	0.47
1:E:85:PHE:CE2	1:E:90:ARG:HB3	2.50	0.47
1:G:220:ILE:HG13	1:G:221:ALA:H	1.80	0.47
1:H:69:GLY:N	1:H:70:PRO:CD	2.73	0.47
1:K:192:GLU:O	1:K:194:TYR:CE1	2.68	0.47
1:K:24:ARG:HD2	1:K:25:PHE:HE2	1.77	0.47
1:B:141:VAL:CG1	1:B:142:THR:N	2.78	0.47
1:D:223:LEU:HD11	1:D:248:ILE:CD1	2.45	0.47
1:E:128:GLY:CA	1:E:134:ILE:HD12	2.42	0.47
1:F:156:ILE:HG22	1:F:159:VAL:HB	1.97	0.47
1:F:16:SER:O	1:F:17:GLU:C	2.53	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:70:PRO:CD	1:F:71:GLN:OE1	2.62	0.47
1:F:77:LYS:N	1:F:77:LYS:HD3	2.29	0.47
1:J:25:PHE:CZ	1:J:213:LYS:HE3	2.50	0.47
1:K:124:ILE:HG21	1:K:173:LEU:HD11	1.96	0.47
1:K:72:ILE:HG12	1:K:103:VAL:CB	2.40	0.47
1:L:107:GLN:HG2	1:L:108:VAL:N	2.30	0.47
1:L:252:MET:HE3	1:L:255:LYS:HD2	1.96	0.47
1:B:212:GLU:O	1:B:268:THR:HB	2.16	0.46
1:F:157:GLY:C	1:F:159:VAL:N	2.67	0.46
1:I:253:LEU:N	1:I:254:PRO:HD2	2.29	0.46
1:J:5:ARG:HH11	1:J:5:ARG:HB2	1.79	0.46
1:L:276:ARG:O	1:L:277:VAL:C	2.52	0.46
1:C:34:TYR:CD2	1:C:35:GLY:N	2.84	0.46
1:E:234:LEU:HB3	1:E:239:VAL:HG23	1.97	0.46
1:E:35:GLY:C	1:E:39:MET:HG3	2.36	0.46
1:F:139:LEU:HD12	1:F:161:GLU:CG	2.45	0.46
1:F:139:LEU:CD2	1:F:159:VAL:HG12	2.44	0.46
1:J:127:THR:HG22	1:J:183:ALA:HB3	1.97	0.46
1:J:223:LEU:HD22	1:J:248:ILE:HD11	1.92	0.46
1:K:76:LEU:HD23	1:K:99:VAL:HG21	1.97	0.46
1:A:169:LEU:HD11	1:A:173:LEU:HD11	1.97	0.46
1:A:213:LYS:HG2	1:A:269:SER:OG	2.16	0.46
1:A:239:VAL:O	1:A:243:ILE:HG13	2.15	0.46
1:G:127:THR:HG23	1:H:110:LYS:HE3	1.98	0.46
1:J:30:LEU:HD12	1:J:60:ILE:HG23	1.95	0.46
1:J:40:GLU:H	1:J:40:GLU:HG3	1.54	0.46
1:L:124:ILE:HG22	1:L:126:LEU:HG	1.97	0.46
1:H:54:LEU:HD21	1:L:15:LEU:HB3	1.97	0.46
1:L:19:LEU:O	1:L:21:TYR:N	2.48	0.46
1:A:224:MET:CA	1:A:229:GLN:O	2.61	0.46
1:A:234:LEU:HD23	1:A:239:VAL:CG2	2.42	0.46
1:E:34:TYR:CD1	1:E:217:LEU:HD12	2.49	0.46
1:F:175:LYS:CD	1:F:175:LYS:N	2.78	0.46
1:G:75:LEU:C	1:G:79:LEU:HD12	2.36	0.46
1:K:40:GLU:OE2	1:K:70:PRO:HB2	2.15	0.46
1:L:4:SER:HB2	1:L:6:ASP:OD2	2.16	0.46
1:B:11:VAL:CG2	1:C:14:VAL:CG1	2.93	0.46
1:C:162:VAL:HB	1:C:204:LYS:HG3	1.97	0.46
1:C:34:TYR:CZ	1:C:39:MET:HB2	2.50	0.46
1:D:41:SER:OG	1:D:42:GLU:N	2.48	0.46
1:E:97:MET:HE1	1:E:195:ASN:CB	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:19:LEU:CB	1:F:20:PRO:HD3	2.45	0.46
1:F:256:ILE:O	1:F:260:LEU:HG	2.14	0.46
1:I:220:ILE:HA	1:I:276:ARG:NH2	2.30	0.46
1:I:225:ASP:C	1:I:227:GLN:N	2.69	0.46
1:J:100:VAL:CG1	1:J:195:ASN:HD21	2.27	0.46
1:J:216:LEU:CD1	1:J:255:LYS:HG2	2.45	0.46
1:J:60:ILE:CD1	1:J:285:ILE:HD13	2.45	0.46
1:K:123:ALA:O	1:L:131:ALA:N	2.48	0.46
1:L:212:GLU:O	1:L:212:GLU:HG3	2.15	0.46
1:L:24:ARG:HG2	1:L:25:PHE:CD1	2.49	0.46
1:C:69:GLY:HA3	1:C:71:GLN:OE1	2.16	0.46
1:E:18:ALA:O	1:E:22:ILE:HG23	2.16	0.46
1:I:128:GLY:HA3	1:I:185:ILE:O	2.14	0.46
1:J:109:ASN:O	1:J:113:VAL:HG23	2.16	0.46
1:J:113:VAL:HG22	1:J:181:VAL:HG21	1.98	0.46
1:K:178:PHE:O	1:K:180:PRO:CD	2.56	0.46
1:L:258:CYS:SG	1:L:259:ALA:N	2.89	0.46
1:L:263:VAL:HG12	1:L:297:ASN:OD1	2.15	0.46
1:L:37:ASN:CG	1:L:38:ALA:N	2.69	0.46
1:B:261:GLU:HA	1:B:264:GLN:HG2	1.98	0.46
1:B:92:THR:HG22	1:B:97:MET:HB2	1.98	0.46
1:D:7:ASP:HA	1:D:10:GLN:HG2	1.97	0.46
1:E:30:LEU:HD11	1:E:213:LYS:CG	2.45	0.46
1:F:92:THR:HG23	1:F:96:THR:HG1	1.81	0.46
1:H:94:ALA:O	1:H:97:MET:HB3	2.16	0.46
1:I:237:GLU:O	1:I:241:GLU:HG3	2.16	0.46
1:L:35:GLY:C	1:L:37:ASN:H	2.17	0.46
1:L:79:LEU:O	1:L:80:SER:HB2	2.16	0.46
1:E:19:LEU:CD2	1:E:22:ILE:HD11	2.46	0.46
1:F:100:VAL:HG11	1:F:195:ASN:ND2	2.30	0.46
1:G:102:MET:HG3	1:H:102:MET:HG3	1.96	0.46
1:G:252:MET:HE1	1:G:272:ILE:HD12	1.98	0.46
1:H:255:LYS:HZ3	3:H:1297:ADP:PB	2.39	0.46
1:H:287:THR:HG22	1:H:288:ASP:N	2.31	0.46
1:J:18:ALA:C	1:J:20:PRO:HD2	2.35	0.46
1:J:236:THR:HG23	1:J:240:ASN:HD21	1.81	0.46
1:K:129:LYS:HZ3	1:K:187:VAL:CG1	2.28	0.46
1:K:274:ASP:C	1:K:276:ARG:H	2.19	0.46
1:K:31:VAL:HG21	1:K:206:ALA:CA	2.44	0.46
1:A:101:GLU:HA	1:A:185:ILE:CD1	2.46	0.46
1:A:113:VAL:HG13	1:A:123:ALA:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:ILE:O	1:A:156:ILE:HG22	2.16	0.46
1:B:60:ILE:HG22	1:B:61:ASN:N	2.30	0.46
1:E:253:LEU:HD12	1:E:253:LEU:HA	1.72	0.46
1:F:23:ARG:O	1:F:24:ARG:C	2.54	0.46
1:F:252:MET:HE3	1:F:255:LYS:HB3	1.97	0.46
1:C:73:GLY:HA3	1:I:224:MET:HE2	1.97	0.46
1:I:255:LYS:HG2	1:I:272:ILE:CD1	2.46	0.46
1:I:3:LEU:HD23	1:I:3:LEU:C	2.37	0.46
1:H:8:ALA:C	1:L:279:ASN:ND2	2.70	0.46
1:B:242:LEU:O	1:B:247:THR:HB	2.16	0.46
1:C:28:LYS:CD	1:C:29:THR:H	2.28	0.46
1:F:13:LYS:HG3	1:F:14:VAL:N	2.30	0.46
1:G:172:MET:HG2	1:H:172:MET:HE2	1.98	0.46
1:I:51:ASP:HB3	1:I:282:LEU:HG	1.98	0.46
1:J:217:LEU:HD23	1:J:273:ILE:HB	1.96	0.46
1:J:279:ASN:OD1	1:K:12:ALA:HB1	2.15	0.46
1:D:271:HIS:ND1	1:D:284:GLU:HG2	2.30	0.45
1:F:184:PRO:CB	1:F:201:VAL:HG21	2.47	0.45
1:F:30:LEU:HD13	1:F:215:MET:HE1	1.98	0.45
1:F:248:ILE:HG21	1:F:256:ILE:HD13	1.98	0.45
1:I:139:LEU:HB2	1:I:161:GLU:HB3	1.98	0.45
1:K:274:ASP:OD1	1:K:276:ARG:CB	2.64	0.45
1:A:136:ALA:HA	1:A:163:THR:HG23	1.98	0.45
1:A:272:ILE:HB	1:A:293:THR:HB	1.98	0.45
1:A:36:GLY:N	1:A:39:MET:HG2	2.30	0.45
1:B:225:ASP:HB3	1:B:231:LEU:HD11	1.98	0.45
1:B:71:GLN:HG2	1:B:107:GLN:NE2	2.28	0.45
1:B:54:LEU:CG	1:C:15:LEU:HD23	2.45	0.45
1:E:136:ALA:CB	1:E:161:GLU:O	2.64	0.45
1:H:196:ILE:CG2	1:H:197:ASN:H	2.28	0.45
1:H:212:GLU:C	1:H:213:LYS:HG2	2.36	0.45
1:G:19:LEU:HD11	1:I:53:VAL:HG12	1.98	0.45
1:J:220:ILE:HD11	3:J:1298:ADP:C3'	2.44	0.45
1:J:72:ILE:HD11	1:J:100:VAL:HA	1.98	0.45
1:A:15:LEU:HB2	1:E:54:LEU:HD21	1.98	0.45
1:E:139:LEU:HD12	1:E:161:GLU:HG2	1.98	0.45
1:F:154:ILE:HG22	1:F:156:ILE:HG13	1.98	0.45
1:G:190:ASN:HB2	1:G:192:GLU:CD	2.36	0.45
1:I:25:PHE:CD1	1:I:285:ILE:HG23	2.52	0.45
1:J:19:LEU:HD12	1:J:22:ILE:HD12	1.97	0.45
1:J:92:THR:CG2	1:J:93:ASP:N	2.78	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:8:ALA:O	1:L:9:ALA:C	2.54	0.45
1:A:234:LEU:CD2	1:A:239:VAL:CG2	2.91	0.45
1:A:31:VAL:HG21	1:A:206:ALA:HB2	1.98	0.45
1:B:28:LYS:HB3	1:B:212:GLU:HB2	1.97	0.45
1:E:242:LEU:HB3	1:E:248:ILE:HG13	1.99	0.45
1:G:141:VAL:HG12	1:G:142:THR:N	2.32	0.45
1:G:236:THR:HG22	1:G:240:ASN:ND2	2.30	0.45
1:H:270:ALA:C	1:H:271:HIS:HD2	2.20	0.45
1:J:23:ARG:NH2	1:K:53:VAL:HG12	2.31	0.45
1:A:294:LEU:HG	1:A:294:LEU:O	2.16	0.45
1:A:29:THR:HA	1:A:61:ASN:O	2.16	0.45
1:C:71:GLN:OE1	1:C:71:GLN:N	2.46	0.45
1:G:279:ASN:O	1:G:283:LEU:HG	2.16	0.45
1:G:39:MET:HE1	1:G:44:LEU:HD23	1.93	0.45
1:H:217:LEU:HD12	1:H:273:ILE:O	2.16	0.45
1:H:225:ASP:CB	1:H:231:LEU:HD21	2.46	0.45
1:I:19:LEU:HA	1:I:19:LEU:HD12	1.60	0.45
1:J:28:LYS:HD2	1:J:28:LYS:HA	1.47	0.45
1:K:127:THR:CG2	1:K:183:ALA:HB3	2.25	0.45
1:L:112:ILE:O	1:L:115:LEU:HB3	2.16	0.45
1:A:207:GLU:O	1:A:210:LYS:HE2	2.16	0.45
1:C:218:THR:OG1	1:C:219:ASN:N	2.50	0.45
1:D:31:VAL:HG21	1:D:206:ALA:HA	1.99	0.45
1:H:234:LEU:HD21	1:H:242:LEU:HD11	1.98	0.45
1:I:195:ASN:ND2	2:I:1300:NLG:H8C1	2.31	0.45
1:I:85:PHE:CE2	1:I:90:ARG:HB3	2.52	0.45
1:K:58:VAL:HG12	1:K:60:ILE:HG13	1.98	0.45
1:K:90:ARG:HH11	1:K:90:ARG:HG3	1.81	0.45
1:B:34:TYR:HD1	1:B:48:PHE:CE1	2.35	0.45
1:D:115:LEU:HA	1:D:115:LEU:HD12	1.75	0.45
1:G:141:VAL:HG11	1:G:156:ILE:CD1	2.46	0.45
1:H:295:ILE:HG23	1:H:296:SER:N	2.31	0.45
1:H:48:PHE:O	1:H:52:VAL:HG23	2.17	0.45
1:I:232:THR:HG22	1:I:294:LEU:HB3	1.99	0.45
1:I:93:ASP:OD1	1:I:96:THR:HG23	2.16	0.45
1:J:34:TYR:CG	1:J:35:GLY:N	2.85	0.45
1:K:109:ASN:HD22	1:K:110:LYS:N	2.12	0.45
1:K:66:HIS:O	1:K:184:PRO:HD3	2.16	0.45
1:C:199:ASP:OD1	1:C:255:LYS:HE2	2.17	0.45
1:F:195:ASN:HD21	2:F:1300:NLG:HBC1	1.81	0.45
1:F:218:THR:CG2	1:F:220:ILE:O	2.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:30:LEU:HD23	1:G:55:MET:HE3	1.99	0.45
1:G:75:LEU:HD23	1:G:99:VAL:HG13	1.99	0.45
1:J:53:VAL:HG11	1:J:119:HIS:O	2.17	0.45
1:A:235:SER:HA	1:A:296:SER:O	2.16	0.45
1:B:135:ARG:NH1	1:B:164:GLY:HA3	2.32	0.45
1:C:271:HIS:ND1	1:C:294:LEU:HD13	2.32	0.45
1:C:5:ARG:H	1:C:5:ARG:HD2	1.81	0.45
1:E:85:PHE:CZ	1:E:90:ARG:CZ	2.99	0.45
1:G:84:HIS:CD2	1:G:84:HIS:O	2.70	0.45
1:H:39:MET:C	1:H:41:SER:H	2.21	0.45
1:I:256:ILE:HD13	1:I:272:ILE:HD11	1.98	0.45
1:J:234:LEU:HA	1:J:238:GLN:OE1	2.17	0.45
1:K:72:ILE:CG1	1:K:103:VAL:HG11	2.46	0.45
1:K:103:VAL:HG13	1:K:107:GLN:NE2	2.30	0.45
1:K:213:LYS:HZ2	1:K:271:HIS:CE1	2.35	0.45
1:K:58:VAL:CG1	1:K:58:VAL:O	2.65	0.45
1:L:162:VAL:HG11	1:L:204:LYS:CB	2.46	0.45
1:A:207:GLU:OE1	1:A:265:GLY:HA3	2.17	0.45
1:B:14:VAL:HG13	1:B:15:LEU:N	2.32	0.45
1:E:125:GLY:O	1:E:126:LEU:HD23	2.16	0.45
1:G:167:VAL:HG23	1:G:167:VAL:O	2.17	0.45
1:G:220:ILE:HG13	1:G:221:ALA:N	2.32	0.45
1:J:124:ILE:HG22	1:J:124:ILE:O	2.17	0.45
1:K:129:LYS:CD	1:K:187:VAL:CG2	2.76	0.45
1:L:4:SER:HB2	1:L:6:ASP:H	1.82	0.45
1:A:21:TYR:HD2	1:A:24:ARG:HE	1.65	0.44
1:A:4:SER:O	1:A:7:ASP:CB	2.64	0.44
1:C:273:ILE:HG12	1:C:274:ASP:H	1.82	0.44
1:F:92:THR:CG2	1:F:96:THR:OG1	2.62	0.44
1:K:226:LYS:HG3	1:K:226:LYS:O	2.16	0.44
1:L:235:SER:OG	1:L:238:GLN:HG3	2.17	0.44
1:L:75:LEU:HD12	1:L:75:LEU:HA	1.69	0.44
1:B:37:ASN:HB2	1:B:219:ASN:ND2	2.32	0.44
1:C:134:ILE:HG22	1:C:134:ILE:O	2.16	0.44
1:C:225:ASP:O	1:C:227:GLN:N	2.50	0.44
1:E:169:LEU:HD12	1:E:172:MET:HE2	1.98	0.44
1:G:118:ARG:CB	1:G:118:ARG:HH11	2.29	0.44
1:G:172:MET:HE3	1:H:172:MET:CG	2.41	0.44
1:G:66:HIS:ND1	1:G:66:HIS:C	2.69	0.44
1:G:85:PHE:O	1:G:86:ILE:O	2.36	0.44
1:H:86:ILE:HG22	1:H:87:ASP:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:167:VAL:HG11	1:I:208:ALA:O	2.16	0.44
1:I:224:MET:HE3	1:I:228:GLY:C	2.37	0.44
1:J:60:ILE:CD1	1:J:285:ILE:CD1	2.95	0.44
1:L:52:VAL:HG12	1:L:179:ILE:HD13	1.99	0.44
1:B:143:ARG:HD3	1:B:152:GLU:HB2	1.99	0.44
1:B:29:THR:O	1:B:211:ALA:HB1	2.18	0.44
1:C:74:ASP:OD1	1:I:220:ILE:HG13	2.17	0.44
1:F:199:ASP:C	1:F:258:CYS:SG	2.96	0.44
1:H:41:SER:C	1:H:43:GLU:N	2.71	0.44
1:J:15:LEU:CD1	1:K:15:LEU:CD1	2.88	0.44
1:K:130:ASP:C	1:K:132:GLU:N	2.70	0.44
1:L:128:GLY:HA3	1:L:134:ILE:HB	1.98	0.44
1:H:3:LEU:HD21	1:L:283:LEU:HD23	1.98	0.44
1:A:86:ILE:CG2	1:A:87:ASP:N	2.73	0.44
1:B:52:VAL:HA	1:B:55:MET:CE	2.46	0.44
1:B:72:ILE:HD11	1:B:104:LEU:CG	2.47	0.44
1:G:55:MET:HG2	1:G:285:ILE:CD1	2.46	0.44
1:G:75:LEU:O	1:G:79:LEU:HD12	2.16	0.44
1:I:60:ILE:C	1:I:62:PRO:HD3	2.37	0.44
1:J:22:ILE:HG23	1:J:58:VAL:CG1	2.47	0.44
1:K:277:VAL:O	1:K:280:ALA:HB2	2.16	0.44
1:L:101:GLU:HA	1:L:185:ILE:CD1	2.47	0.44
1:B:58:VAL:HG12	1:B:60:ILE:HD12	1.98	0.44
1:C:217:LEU:N	1:C:217:LEU:HD23	2.32	0.44
1:C:226:LYS:CG	1:C:247:THR:HB	2.47	0.44
1:F:289:SER:OG	1:F:290:GLY:N	2.51	0.44
1:I:253:LEU:N	1:I:254:PRO:CD	2.81	0.44
1:J:252:MET:HE1	1:J:255:LYS:HD2	1.96	0.44
1:L:22:ILE:HG12	1:L:58:VAL:HG11	1.99	0.44
1:L:38:ALA:C	1:L:40:GLU:N	2.70	0.44
1:B:25:PHE:CE1	1:B:285:ILE:HD12	2.52	0.44
1:D:252:MET:HG3	1:D:252:MET:O	2.18	0.44
1:F:17:GLU:O	1:F:20:PRO:HD2	2.17	0.44
1:F:199:ASP:O	1:F:258:CYS:SG	2.75	0.44
1:G:55:MET:HE1	1:G:62:PRO:HB3	1.98	0.44
1:H:218:THR:OG1	1:H:219:ASN:N	2.49	0.44
1:J:72:ILE:HG13	1:J:103:VAL:HG11	1.99	0.44
1:L:211:ALA:O	1:L:267:VAL:HG13	2.17	0.44
1:L:22:ILE:CG1	1:L:58:VAL:HG11	2.48	0.44
1:A:10:GLN:O	1:A:14:VAL:CG2	2.66	0.44
1:A:30:LEU:CD1	1:A:55:MET:CE	2.96	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:229:GLN:NE2	1:B:229:GLN:HA	2.31	0.44
1:C:2:THR:HG22	1:C:3:LEU:N	2.23	0.44
1:F:219:ASN:ND2	1:F:219:ASN:N	2.63	0.44
1:F:213:LYS:HA	1:F:269:SER:O	2.17	0.44
1:G:39:MET:HE1	1:G:44:LEU:CD2	2.47	0.44
1:H:90:ARG:HD3	1:H:96:THR:CG2	2.48	0.44
1:I:223:LEU:C	1:I:223:LEU:CD1	2.71	0.44
1:I:256:ILE:HD12	1:I:295:ILE:CD1	2.43	0.44
1:I:239:VAL:HG21	1:I:256:ILE:HG21	2.00	0.44
1:C:43:GLU:OE1	1:I:84:HIS:HA	2.18	0.44
1:J:160:GLY:O	1:J:196:ILE:HG12	2.17	0.44
1:J:220:ILE:HD12	3:J:1298:ADP:C2'	2.43	0.44
1:L:200:LEU:O	1:L:204:LYS:HG2	2.17	0.44
1:A:114:ASN:O	1:A:117:ASN:HB2	2.18	0.44
1:A:23:ARG:CG	1:A:23:ARG:NH1	2.78	0.44
1:A:231:LEU:CD2	1:A:242:LEU:HD21	2.44	0.44
1:B:25:PHE:CD2	1:B:212:GLU:HG2	2.49	0.44
1:B:232:THR:HG22	1:B:233:GLY:H	1.83	0.44
1:F:125:GLY:O	1:F:126:LEU:HD23	2.18	0.44
1:F:58:VAL:O	1:F:58:VAL:HG12	2.17	0.44
1:F:89:MET:SD	1:F:139:LEU:CD2	3.01	0.44
1:G:79:LEU:O	1:G:80:SER:CB	2.60	0.44
1:J:220:ILE:CD1	3:J:1298:ADP:H2'	2.47	0.44
1:J:66:HIS:O	1:J:184:PRO:HD3	2.18	0.44
1:J:60:ILE:HD11	1:J:285:ILE:HD13	2.00	0.44
1:L:220:ILE:HD13	3:L:1300:ADP:N3	2.33	0.44
1:A:33:LYS:HA	1:A:65:VAL:O	2.18	0.44
1:C:21:TYR:HD2	1:C:24:ARG:NH1	2.15	0.44
1:E:19:LEU:O	1:E:22:ILE:HG12	2.18	0.44
1:F:220:ILE:O	1:F:222:GLY:N	2.51	0.44
1:G:28:LYS:HA	1:G:28:LYS:HD2	1.78	0.44
1:G:36:GLY:O	1:G:39:MET:HB3	2.17	0.44
1:H:97:MET:HE1	1:H:195:ASN:HB2	1.96	0.44
1:I:167:VAL:HG13	1:I:208:ALA:HB1	2.00	0.44
1:K:75:LEU:HA	1:K:75:LEU:HD12	1.72	0.44
1:L:141:VAL:O	1:L:153:ILE:HG23	2.17	0.44
1:C:102:MET:HG3	1:D:107:GLN:HB2	2.01	0.43
1:C:196:ILE:HG22	1:C:197:ASN:N	2.32	0.43
1:D:32:ILE:HD11	1:D:55:MET:HE1	1.99	0.43
1:J:225:ASP:O	1:J:225:ASP:OD1	2.36	0.43
1:K:33:LYS:HB2	1:K:202:ALA:CB	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:72:ILE:HD11	1:K:104:LEU:CG	2.34	0.43
1:H:120:GLY:HA3	1:L:23:ARG:HD2	2.00	0.43
1:A:170:LEU:HD23	1:A:170:LEU:HA	1.86	0.43
1:B:252:MET:CE	1:B:255:LYS:HB3	2.47	0.43
1:B:58:VAL:HG12	1:B:60:ILE:CD1	2.48	0.43
1:F:239:VAL:HB	1:F:260:LEU:HD21	2.00	0.43
1:G:252:MET:CE	1:G:256:ILE:HG13	2.46	0.43
1:G:32:ILE:HD11	1:G:55:MET:HE1	2.00	0.43
1:H:69:GLY:HA3	2:H:1299:NLG:O	2.18	0.43
1:K:129:LYS:HE2	1:L:114:ASN:HA	2.00	0.43
1:C:249:TYR:O	3:C:1300:ADP:H8	2.00	0.43
1:C:34:TYR:OH	1:C:39:MET:HB2	2.19	0.43
1:E:217:LEU:CD2	1:E:273:ILE:HD11	2.48	0.43
1:F:196:ILE:O	2:F:1300:NLG:HBC2	2.19	0.43
1:H:212:GLU:O	1:H:213:LYS:HD3	2.19	0.43
1:H:232:THR:CG2	1:H:233:GLY:N	2.57	0.43
1:H:252:MET:CG	3:H:1297:ADP:C4	3.01	0.43
1:L:271:HIS:NE2	1:L:284:GLU:OE2	2.47	0.43
1:C:15:LEU:O	1:C:19:LEU:N	2.51	0.43
1:D:75:LEU:HA	1:D:75:LEU:HD12	1.83	0.43
1:A:14:VAL:HG11	1:E:11:VAL:HG22	2.00	0.43
1:F:113:VAL:HG12	1:F:114:ASN:N	2.32	0.43
1:F:11:VAL:O	1:F:15:LEU:CG	2.56	0.43
1:H:276:ARG:O	1:H:278:PRO:HD3	2.18	0.43
1:I:262:ALA:O	1:I:267:VAL:N	2.51	0.43
1:J:51:ASP:O	1:J:54:LEU:HB3	2.19	0.43
1:J:5:ARG:NH1	1:J:5:ARG:HB2	2.33	0.43
1:K:262:ALA:HB1	1:K:267:VAL:HG21	2.01	0.43
1:L:60:ILE:CG2	1:L:61:ASN:N	2.81	0.43
1:A:141:VAL:HG21	1:A:156:ILE:HG13	2.00	0.43
1:A:30:LEU:HD21	1:A:213:LYS:HG3	2.00	0.43
1:B:30:LEU:HD21	1:B:215:MET:CE	2.48	0.43
1:C:274:ASP:OD1	1:C:276:ARG:HB2	2.18	0.43
1:D:3:LEU:HB3	1:F:21:TYR:CE1	2.53	0.43
1:F:244:ALA:C	1:F:246:GLY:H	2.21	0.43
1:J:236:THR:CG2	1:J:240:ASN:ND2	2.82	0.43
1:K:44:LEU:HD21	1:K:276:ARG:HA	2.00	0.43
1:A:13:LYS:HA	1:A:16:SER:HB2	2.01	0.43
1:A:232:THR:CG2	1:A:290:GLY:O	2.67	0.43
1:B:235:SER:H	1:B:238:GLN:HG3	1.83	0.43
1:A:16:SER:HB3	1:E:50:ARG:CZ	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:89:MET:HB3	2:F:1300:NLG:H8C2	2.00	0.43
1:G:224:MET:HE3	1:G:228:GLY:C	2.39	0.43
1:H:139:LEU:HB3	1:H:159:VAL:O	2.19	0.43
1:I:210:LYS:HE3	1:I:266:GLY:HA2	1.99	0.43
1:I:232:THR:CG2	1:I:294:LEU:H	2.30	0.43
1:B:176:GLY:O	1:B:177:ASP:HB2	2.18	0.43
1:B:218:THR:OG1	1:B:219:ASN:N	2.46	0.43
1:C:255:LYS:O	1:C:258:CYS:HB2	2.18	0.43
1:E:231:LEU:HD12	1:E:234:LEU:HD11	2.01	0.43
1:E:60:ILE:O	1:E:62:PRO:HD3	2.19	0.43
1:F:13:LYS:CG	1:F:14:VAL:N	2.82	0.43
1:F:238:GLN:HA	1:F:241:GLU:CD	2.39	0.43
1:G:10:GLN:O	1:G:14:VAL:HG23	2.19	0.43
1:H:183:ALA:HA	1:H:184:PRO:HD3	1.79	0.43
1:I:65:VAL:HG21	1:I:202:ALA:CA	2.47	0.43
1:J:188:GLY:CA	1:J:192:GLU:OE2	2.65	0.43
1:J:28:LYS:CB	1:J:212:GLU:HB2	2.49	0.43
1:J:46:ALA:O	1:J:49:ALA:HB3	2.19	0.43
1:L:113:VAL:HG13	1:L:117:ASN:HD21	1.83	0.43
1:L:135:ARG:NH1	1:L:164:GLY:HA3	2.34	0.43
1:A:43:GLU:HG3	1:A:43:GLU:H	1.59	0.43
1:D:3:LEU:HD12	1:F:287:THR:HG23	2.00	0.43
1:E:13:LYS:NZ	1:E:17:GLU:OE2	2.51	0.43
1:F:277:VAL:O	1:F:280:ALA:HB2	2.18	0.43
1:G:232:THR:CG2	1:G:233:GLY:N	2.81	0.43
1:H:145:THR:O	1:H:147:GLU:N	2.46	0.43
1:H:52:VAL:O	1:H:55:MET:HB2	2.19	0.43
1:H:55:MET:HE1	1:H:285:ILE:HD12	2.00	0.43
1:I:33:LYS:HA	1:I:65:VAL:O	2.18	0.43
1:J:12:ALA:HB1	1:K:282:LEU:HD12	1.96	0.43
1:L:72:ILE:O	1:L:76:LEU:CG	2.60	0.43
1:L:72:ILE:HG22	1:L:90:ARG:NH2	2.34	0.43
1:C:242:LEU:HA	1:C:242:LEU:HD23	1.90	0.43
1:F:77:LYS:H	1:F:77:LYS:HD3	1.84	0.43
1:G:141:VAL:HG12	1:G:142:THR:H	1.82	0.43
1:H:156:ILE:O	1:H:156:ILE:HG22	2.18	0.43
1:J:101:GLU:HA	1:J:185:ILE:CD1	2.48	0.43
1:J:35:GLY:O	1:J:39:MET:HE1	2.13	0.43
1:L:139:LEU:HD12	1:L:140:THR:H	1.82	0.43
1:L:237:GLU:CD	1:L:237:GLU:N	2.72	0.43
1:A:285:ILE:C	1:A:287:THR:N	2.71	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:215:MET:SD	1:C:281:VAL:CG2	3.04	0.43
1:E:167:VAL:CG1	1:E:171:ASN:ND2	2.75	0.43
1:E:76:LEU:HD23	1:E:83:SER:HB3	2.00	0.43
1:F:261:GLU:O	1:F:262:ALA:C	2.57	0.43
1:F:70:PRO:N	1:F:71:GLN:OE1	2.52	0.43
1:H:12:ALA:O	1:H:16:SER:HB3	2.18	0.43
1:I:224:MET:CE	1:I:228:GLY:HA2	2.49	0.43
1:I:273:ILE:CD1	1:I:284:GLU:CG	2.76	0.43
1:K:72:ILE:HD13	1:K:100:VAL:HG22	2.01	0.43
1:L:223:LEU:CD1	1:L:256:ILE:HD13	2.45	0.43
1:L:22:ILE:HG21	1:L:58:VAL:CG1	2.49	0.43
1:A:38:ALA:HB3	1:A:219:ASN:OD1	2.19	0.42
1:D:143:ARG:HA	1:D:143:ARG:HD2	1.60	0.42
1:F:128:GLY:HA3	1:F:185:ILE:O	2.18	0.42
1:I:86:ILE:HD13	1:I:154:ILE:CD1	2.49	0.42
1:I:39:MET:HA	1:I:44:LEU:HD22	2.00	0.42
1:J:252:MET:SD	3:J:1298:ADP:C2	3.12	0.42
1:J:252:MET:HE3	1:J:255:LYS:HD2	1.95	0.42
1:J:30:LEU:HD22	1:J:215:MET:HE1	1.97	0.42
1:L:30:LEU:CD1	1:L:285:ILE:HD11	2.49	0.42
1:A:21:TYR:O	1:A:24:ARG:N	2.52	0.42
1:C:33:LYS:HD3	1:C:33:LYS:C	2.39	0.42
1:B:282:LEU:CD2	1:C:8:ALA:HB1	2.49	0.42
1:D:209:LEU:O	1:D:210:LYS:C	2.56	0.42
1:E:162:VAL:CB	1:E:204:LYS:HG3	2.42	0.42
1:F:52:VAL:CG1	1:F:179:ILE:HD13	2.50	0.42
1:G:252:MET:CE	1:G:255:LYS:HD2	2.48	0.42
1:H:232:THR:HG23	1:H:294:LEU:O	2.19	0.42
1:H:28:LYS:HD3	1:H:28:LYS:N	2.34	0.42
1:I:19:LEU:O	1:I:20:PRO:C	2.56	0.42
1:G:283:LEU:HD21	1:I:8:ALA:CB	2.48	0.42
1:J:15:LEU:HD13	1:K:15:LEU:CG	2.49	0.42
1:J:55:MET:HA	1:J:60:ILE:HD12	2.01	0.42
1:L:30:LEU:HD12	1:L:55:MET:HE3	2.01	0.42
1:L:35:GLY:C	1:L:37:ASN:N	2.72	0.42
1:L:96:THR:O	1:L:100:VAL:HG23	2.19	0.42
1:A:11:VAL:HG23	1:E:14:VAL:HG13	1.97	0.42
1:A:242:LEU:HA	1:A:242:LEU:HD13	1.85	0.42
1:A:218:THR:CG2	1:A:255:LYS:HE3	2.45	0.42
1:B:137:LYS:H	1:B:163:THR:HG23	1.83	0.42
1:G:101:GLU:OE1	1:G:129:LYS:HE3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:154:ILE:HG23	1:L:154:ILE:O	2.18	0.42
1:L:51:ASP:OD1	1:L:282:LEU:HD12	2.19	0.42
1:A:172:MET:HE1	1:B:173:LEU:HD23	2.02	0.42
1:B:30:LEU:O	1:B:62:PRO:HA	2.19	0.42
1:C:73:GLY:HA3	1:I:224:MET:CE	2.48	0.42
1:F:85:PHE:CD1	1:F:86:ILE:N	2.87	0.42
1:F:85:PHE:CE2	1:F:90:ARG:HD3	2.55	0.42
1:H:212:GLU:OE2	1:H:213:LYS:HE2	2.19	0.42
1:L:60:ILE:O	1:L:62:PRO:HD3	2.19	0.42
1:A:167:VAL:CG1	1:A:171:ASN:ND2	2.83	0.42
1:A:221:ALA:HA	1:A:274:ASP:OD2	2.19	0.42
1:A:29:THR:HG21	1:A:209:LEU:HD13	2.01	0.42
1:B:109:ASN:HD21	1:B:125:GLY:HA3	1.84	0.42
1:B:50:ARG:HH21	1:B:279:ASN:HD21	1.67	0.42
1:D:297:ASN:HB3	1:D:298:ARG:H	1.71	0.42
1:D:58:VAL:O	1:D:58:VAL:CG1	2.66	0.42
1:H:34:TYR:CG	1:H:35:GLY:N	2.85	0.42
1:J:222:GLY:O	1:J:223:LEU:C	2.58	0.42
1:J:225:ASP:OD2	1:J:229:GLN:CB	2.63	0.42
1:K:18:ALA:O	1:K:19:LEU:C	2.57	0.42
1:L:270:ALA:HB3	1:L:295:ILE:HB	2.01	0.42
1:B:115:LEU:HA	1:B:115:LEU:HD12	1.87	0.42
1:B:251:GLY:HA3	3:B:1300:ADP:O2A	2.20	0.42
1:D:196:ILE:HG22	1:D:197:ASN:N	2.35	0.42
1:G:11:VAL:CG2	1:I:14:VAL:HG12	2.50	0.42
1:H:259:ALA:O	1:H:263:VAL:CG2	2.67	0.42
1:I:8:ALA:O	1:I:11:VAL:HB	2.19	0.42
1:I:256:ILE:HD13	1:I:272:ILE:CD1	2.50	0.42
1:J:247:THR:O	3:J:1298:ADP:N6	2.44	0.42
1:K:10:GLN:O	1:K:14:VAL:HG23	2.19	0.42
1:K:198:ALA:N	2:K:1298:NLG:OE1	2.49	0.42
1:L:55:MET:HB3	1:L:60:ILE:HB	2.01	0.42
1:B:142:THR:CG2	1:B:143:ARG:N	2.83	0.42
1:C:141:VAL:HG21	1:C:156:ILE:CD1	2.49	0.42
1:F:37:ASN:N	1:F:37:ASN:ND2	2.66	0.42
1:H:206:ALA:HB3	1:H:214:LEU:HD22	2.01	0.42
1:J:37:ASN:C	1:J:39:MET:N	2.71	0.42
1:I:102:MET:HE1	1:J:75:LEU:CD2	2.50	0.42
1:K:129:LYS:HE2	1:L:114:ASN:ND2	2.34	0.42
1:B:4:SER:O	1:B:7:ASP:HB2	2.20	0.42
1:B:72:ILE:O	1:B:76:LEU:HD22	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:217:LEU:HD22	1:C:273:ILE:HG23	2.00	0.42
1:E:136:ALA:HB1	1:E:161:GLU:O	2.20	0.42
1:H:5:ARG:CG	1:H:6:ASP:N	2.83	0.42
1:H:90:ARG:HD3	1:H:96:THR:HG21	2.01	0.42
1:J:253:LEU:CB	1:J:254:PRO:CD	2.93	0.42
1:K:101:GLU:HA	1:K:185:ILE:HD13	2.01	0.42
1:K:129:LYS:HD2	1:K:129:LYS:HA	1.73	0.42
1:K:277:VAL:CG1	1:K:278:PRO:HD2	2.49	0.42
1:K:90:ARG:HG3	1:K:90:ARG:NH1	2.35	0.42
1:L:22:ILE:HD11	1:L:286:PHE:CZ	2.55	0.42
1:L:263:VAL:CG1	1:L:297:ASN:HB2	2.50	0.42
1:L:32:ILE:HD11	1:L:55:MET:CE	2.49	0.42
1:L:76:LEU:HD23	1:L:99:VAL:HG21	2.02	0.42
1:D:35:GLY:C	1:D:37:ASN:N	2.72	0.42
1:E:22:ILE:HG22	1:E:286:PHE:HD1	1.81	0.42
1:E:34:TYR:CD2	1:E:35:GLY:N	2.86	0.42
1:E:97:MET:CE	1:E:158:HIS:O	2.68	0.42
1:F:29:THR:HG21	1:F:209:LEU:HD13	2.01	0.42
1:F:30:LEU:HD13	1:F:215:MET:CE	2.49	0.42
1:G:199:ASP:OD1	1:G:255:LYS:HG3	2.19	0.42
1:G:34:TYR:OH	1:G:45:LYS:HG3	2.20	0.42
1:H:220:ILE:HG21	3:H:1297:ADP:H3'	2.01	0.42
1:H:55:MET:HB3	1:H:55:MET:HE2	1.97	0.42
1:I:260:LEU:O	1:I:264:GLN:HB2	2.20	0.42
1:I:3:LEU:HG	1:I:7:ASP:HB3	2.01	0.42
1:L:245:ASP:HB3	1:L:247:THR:OG1	2.20	0.42
1:A:237:GLU:HA	1:A:237:GLU:OE1	2.20	0.42
1:B:215:MET:SD	1:B:284:GLU:HG2	2.60	0.42
1:D:252:MET:HE3	1:D:252:MET:HA	2.02	0.42
1:F:251:GLY:HA3	3:F:1299:ADP:O2A	2.19	0.42
1:F:138:LYS:HE3	1:F:157:GLY:CA	2.32	0.42
1:F:259:ALA:O	1:F:262:ALA:HB3	2.20	0.42
1:G:115:LEU:HD12	1:G:115:LEU:HA	1.79	0.42
1:G:56:LYS:HE2	1:G:177:ASP:HA	2.01	0.42
1:I:99:VAL:HG12	1:I:100:VAL:N	2.34	0.42
1:K:15:LEU:HA	1:K:15:LEU:HD23	1.77	0.42
1:K:271:HIS:NE2	1:K:294:LEU:HD12	2.34	0.42
1:K:217:LEU:HD22	1:K:275:GLY:HA2	2.02	0.42
1:B:42:GLU:OE1	1:B:45:LYS:NZ	2.52	0.41
1:D:22:ILE:CG2	1:D:58:VAL:HG13	2.50	0.41
1:D:30:LEU:HD22	1:D:213:LYS:CB	2.44	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:89:MET:HE2	1:D:159:VAL:CG1	2.50	0.41
1:F:133:LEU:O	1:F:165:VAL:HA	2.19	0.41
1:G:66:HIS:CD2	1:G:112:ILE:HD12	2.55	0.41
1:H:126:LEU:HD11	1:H:173:LEU:HD11	2.02	0.41
1:H:213:LYS:HD3	1:H:269:SER:HG	1.85	0.41
1:I:155:ASP:CG	1:I:155:ASP:O	2.58	0.41
1:K:37:ASN:O	1:K:39:MET:N	2.53	0.41
1:A:77:LYS:HE2	1:A:77:LYS:HB2	1.80	0.41
1:B:170:LEU:HA	1:B:170:LEU:HD23	1.85	0.41
1:D:166:ASN:C	1:D:166:ASN:OD1	2.59	0.41
1:K:271:HIS:CD2	1:K:271:HIS:N	2.87	0.41
1:L:232:THR:HG23	1:L:294:LEU:N	2.28	0.41
1:L:252:MET:HE3	1:L:255:LYS:CB	2.48	0.41
1:L:30:LEU:HD12	1:L:55:MET:SD	2.60	0.41
1:B:19:LEU:N	1:B:20:PRO:CD	2.83	0.41
1:D:231:LEU:O	1:D:293:THR:HG23	2.20	0.41
1:E:113:VAL:HG22	1:E:123:ALA:CB	2.50	0.41
1:E:256:ILE:HD12	1:E:257:ARG:HG3	2.02	0.41
1:G:11:VAL:HG23	1:I:14:VAL:HG12	2.02	0.41
1:G:207:GLU:O	1:G:210:LYS:N	2.44	0.41
1:H:100:VAL:HG12	1:H:104:LEU:CD1	2.47	0.41
1:H:92:THR:HG22	1:H:97:MET:HE2	1.96	0.41
1:J:273:ILE:CG2	1:J:274:ASP:N	2.83	0.41
1:K:21:TYR:N	1:K:21:TYR:CD1	2.86	0.41
1:K:262:ALA:O	1:K:267:VAL:HG23	2.21	0.41
1:L:223:LEU:O	1:L:230:VAL:CA	2.68	0.41
1:D:2:THR:O	1:D:2:THR:HG23	2.20	0.41
1:F:219:ASN:HD21	3:F:1299:ADP:H5'1	1.85	0.41
1:G:29:THR:HG22	1:G:211:ALA:CB	2.50	0.41
1:H:141:VAL:HG11	1:H:156:ILE:HD11	2.02	0.41
1:I:81:ILE:HG23	1:I:82:GLU:H	1.85	0.41
1:K:124:ILE:HG22	1:K:126:LEU:CG	2.50	0.41
1:K:24:ARG:HH12	1:K:288:ASP:CA	2.33	0.41
1:A:33:LYS:CE	1:A:199:ASP:OD2	2.64	0.41
1:B:51:ASP:O	1:B:55:MET:HG3	2.20	0.41
1:D:218:THR:HG23	1:D:219:ASN:N	2.35	0.41
1:D:221:ALA:HA	1:D:274:ASP:HB2	2.03	0.41
1:E:274:ASP:OD1	1:E:276:ARG:HB2	2.20	0.41
1:F:213:LYS:HG2	1:F:269:SER:OG	2.21	0.41
1:H:24:ARG:HG3	1:H:25:PHE:CE2	2.55	0.41
1:H:253:LEU:O	1:H:254:PRO:C	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:79:LEU:HB3	1:H:81:ILE:CD1	2.50	0.41
1:K:113:VAL:HG13	1:K:123:ALA:HB3	2.03	0.41
1:H:3:LEU:CD2	1:L:283:LEU:HD23	2.51	0.41
1:L:34:TYR:HA	1:L:217:LEU:HD12	2.02	0.41
1:B:14:VAL:HG11	1:C:11:VAL:HG21	1.95	0.41
1:B:32:ILE:CD1	1:B:52:VAL:HG22	2.50	0.41
1:C:213:LYS:HA	1:C:269:SER:O	2.21	0.41
1:C:273:ILE:CG1	1:C:274:ASP:N	2.82	0.41
1:D:133:LEU:HG	1:D:134:ILE:HG13	2.02	0.41
1:G:156:ILE:CG2	1:G:156:ILE:O	2.68	0.41
1:G:187:VAL:HA	1:G:192:GLU:O	2.20	0.41
1:J:100:VAL:HG12	1:J:104:LEU:HD12	2.02	0.41
1:J:109:ASN:OD1	1:J:125:GLY:HA3	2.21	0.41
1:J:158:HIS:O	1:J:159:VAL:HG23	2.20	0.41
1:J:31:VAL:HG11	1:J:202:ALA:O	2.21	0.41
1:K:195:ASN:ND2	2:K:1298:NLG:O	2.49	0.41
1:K:25:PHE:CD1	1:K:285:ILE:HB	2.55	0.41
1:A:139:LEU:N	1:A:160:GLY:HA2	2.34	0.41
1:A:31:VAL:HG21	1:A:206:ALA:HA	2.02	0.41
1:C:298:ARG:O	1:C:299:LYS:HB2	2.20	0.41
1:C:60:ILE:O	1:C:62:PRO:HD3	2.21	0.41
1:F:89:MET:HE3	1:F:139:LEU:HD23	2.03	0.41
1:H:19:LEU:CD2	1:L:53:VAL:CG1	2.98	0.41
1:K:172:MET:HE2	1:L:172:MET:O	2.21	0.41
1:K:213:LYS:HZ2	1:K:271:HIS:HE1	1.68	0.41
1:L:22:ILE:CG2	1:L:58:VAL:CG1	2.99	0.41
1:G:273:ILE:HG23	1:G:274:ASP:N	2.35	0.41
1:J:11:VAL:HA	1:K:14:VAL:CG1	2.51	0.41
1:K:162:VAL:CB	1:K:204:LYS:HG3	2.51	0.41
1:L:156:ILE:HG22	1:L:159:VAL:CG2	2.40	0.41
1:L:76:LEU:CD1	1:L:90:ARG:NH2	2.83	0.41
1:B:141:VAL:CG1	1:B:142:THR:H	2.34	0.41
1:D:107:GLN:O	1:D:111:ASP:HB3	2.20	0.41
1:K:274:ASP:HB3	1:K:277:VAL:HG23	2.03	0.41
1:K:271:HIS:CE1	1:K:284:GLU:HG3	2.55	0.41
1:L:19:LEU:HB3	1:L:20:PRO:CD	2.44	0.41
1:C:16:SER:O	1:C:19:LEU:HB2	2.20	0.41
1:B:14:VAL:CG2	1:C:3:LEU:HD13	2.50	0.41
1:D:96:THR:O	1:D:100:VAL:HG23	2.21	0.41
1:E:289:SER:HB2	1:E:291:VAL:CG1	2.50	0.41
1:F:219:ASN:N	1:F:219:ASN:HD22	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:144:GLN:O	1:H:146:PRO:HD3	2.20	0.41
1:J:66:HIS:CD2	1:J:112:ILE:HD12	2.56	0.41
1:J:86:ILE:HG23	1:J:87:ASP:N	2.35	0.41
1:K:72:ILE:CG1	1:K:103:VAL:CG1	2.97	0.41
1:A:41:SER:O	1:A:45:LYS:HG3	2.21	0.41
1:D:233:GLY:N	1:D:294:LEU:O	2.54	0.41
1:E:22:ILE:HG22	1:E:286:PHE:CE1	2.56	0.41
1:F:122:SER:HB3	1:F:178:PHE:CD2	2.56	0.41
1:G:89:MET:CB	2:G:1301:NLG:H8C2	2.49	0.41
1:G:273:ILE:CD1	1:G:291:VAL:O	2.67	0.41
1:G:54:LEU:O	1:G:55:MET:C	2.58	0.41
1:I:225:ASP:HB3	1:I:229:GLN:H	1.85	0.41
1:I:55:MET:HE1	1:I:215:MET:CE	2.49	0.41
1:K:173:LEU:HD22	1:K:178:PHE:HB3	2.03	0.41
1:K:282:LEU:HA	1:K:285:ILE:HG12	2.02	0.41
1:L:42:GLU:O	1:L:45:LYS:HB2	2.20	0.41
1:A:15:LEU:CB	1:E:54:LEU:HD21	2.51	0.40
1:A:224:MET:CB	1:A:229:GLN:O	2.69	0.40
1:B:34:TYR:CD2	1:B:35:GLY:N	2.89	0.40
1:B:34:TYR:CE2	1:B:39:MET:HG3	2.56	0.40
1:C:29:THR:HG21	1:C:209:LEU:HD13	2.03	0.40
1:D:252:MET:HE1	1:D:272:ILE:CD1	2.49	0.40
1:D:54:LEU:HD11	1:F:15:LEU:CD1	2.47	0.40
1:E:72:ILE:CD1	1:E:104:LEU:HG	2.49	0.40
1:I:122:SER:HB3	1:I:178:PHE:CD2	2.56	0.40
1:K:39:MET:O	1:K:40:GLU:HB2	2.21	0.40
1:K:76:LEU:HA	1:K:76:LEU:HD23	1.90	0.40
1:H:12:ALA:CB	1:L:50:ARG:HH21	2.28	0.40
1:L:55:MET:SD	1:L:60:ILE:HG21	2.61	0.40
1:B:143:ARG:O	1:B:144:GLN:CG	2.69	0.40
1:D:37:ASN:N	1:D:37:ASN:OD1	2.55	0.40
1:D:58:VAL:O	1:D:58:VAL:HG13	2.21	0.40
1:E:178:PHE:CE2	1:F:169:LEU:HD13	2.56	0.40
1:G:232:THR:HG22	1:G:233:GLY:H	1.86	0.40
1:G:287:THR:HG22	1:G:288:ASP:H	1.85	0.40
1:G:173:LEU:HA	1:H:172:MET:HE1	2.02	0.40
1:I:252:MET:HG3	1:I:252:MET:O	2.21	0.40
1:I:271:HIS:HB3	1:I:273:ILE:CD1	2.51	0.40
1:J:49:ALA:O	1:J:53:VAL:HG23	2.22	0.40
1:K:66:HIS:O	1:K:184:PRO:HG2	2.17	0.40
1:K:81:ILE:HD13	1:K:95:ALA:HB1	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:MET:O	1:A:60:ILE:HG13	2.21	0.40
1:C:72:ILE:HD11	1:C:104:LEU:HD21	2.03	0.40
1:C:251:GLY:O	1:C:254:PRO:HD2	2.21	0.40
1:C:70:PRO:HD2	1:C:71:GLN:NE2	2.36	0.40
1:D:41:SER:O	1:D:42:GLU:HG2	2.21	0.40
1:E:159:VAL:HA	1:E:195:ASN:O	2.22	0.40
1:F:272:ILE:C	1:F:273:ILE:HG13	2.41	0.40
1:G:36:GLY:CA	1:G:39:MET:CB	2.62	0.40
1:H:287:THR:CG2	1:H:288:ASP:N	2.82	0.40
1:I:30:LEU:HD22	1:I:213:LYS:CB	2.48	0.40
1:J:30:LEU:HD23	1:J:213:LYS:HB2	1.96	0.40
1:J:2:THR:O	1:J:3:LEU:HB2	2.21	0.40
1:J:38:ALA:O	1:J:40:GLU:N	2.54	0.40
1:L:60:ILE:HG22	1:L:61:ASN:N	2.36	0.40
1:A:53:VAL:HG21	1:A:119:HIS:O	2.20	0.40
1:A:285:ILE:O	1:A:287:THR:N	2.55	0.40
1:A:31:VAL:HG21	1:A:206:ALA:CB	2.52	0.40
1:B:34:TYR:CD2	1:B:39:MET:HE2	2.56	0.40
1:C:55:MET:CE	1:C:285:ILE:HD13	2.50	0.40
1:C:5:ARG:NH1	1:C:5:ARG:CG	2.84	0.40
1:E:218:THR:CB	1:E:255:LYS:HE2	2.51	0.40
1:G:209:LEU:O	1:G:210:LYS:C	2.59	0.40
1:G:70:PRO:HB2	1:G:71:GLN:OE1	2.21	0.40
1:H:25:PHE:CA	1:H:28:LYS:HG2	2.39	0.40
1:H:8:ALA:C	1:L:279:ASN:HD21	2.25	0.40
1:I:213:LYS:HG3	1:I:269:SER:HG	1.84	0.40
1:I:66:HIS:O	1:I:184:PRO:CD	2.69	0.40
1:K:274:ASP:C	1:K:276:ARG:N	2.74	0.40
1:L:54:LEU:HD11	1:L:286:PHE:HZ	1.87	0.40
1:B:248:ILE:HG23	1:B:252:MET:CG	2.52	0.40
1:A:11:VAL:HG22	1:E:15:LEU:HD23	2.03	0.40
1:E:2:THR:HG23	1:E:4:SER:CA	2.51	0.40
1:E:33:LYS:HE2	1:E:198:ALA:CB	2.52	0.40
1:G:29:THR:HG22	1:G:211:ALA:HB2	2.04	0.40
1:H:145:THR:CG2	1:H:147:GLU:OE2	2.69	0.40
1:H:72:ILE:O	1:H:76:LEU:HG	2.21	0.40
1:I:232:THR:HG23	1:I:294:LEU:N	2.32	0.40
1:I:271:HIS:CE1	1:I:294:LEU:HD22	2.56	0.40
1:I:284:GLU:HA	1:I:284:GLU:OE1	2.21	0.40
1:I:56:LYS:HD2	1:I:56:LYS:HA	1.85	0.40
1:J:128:GLY:HA3	1:J:185:ILE:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:34:TYR:CE1	1:J:48:PHE:CG	3.09	0.40
1:J:86:ILE:HB	1:J:91:VAL:CG2	2.51	0.40
1:K:19:LEU:HA	1:K:22:ILE:HD12	2.03	0.40
1:K:129:LYS:HE2	1:L:114:ASN:CB	2.51	0.40
1:L:232:THR:O	1:L:233:GLY:C	2.60	0.40
1:L:91:VAL:HA	1:L:156:ILE:O	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	288/300 (96%)	249 (86%)	34 (12%)	5 (2%)	9	34
1	B	293/300 (98%)	268 (92%)	23 (8%)	2 (1%)	22	56
1	C	297/300 (99%)	272 (92%)	20 (7%)	5 (2%)	9	34
1	D	291/300 (97%)	272 (94%)	14 (5%)	5 (2%)	9	34
1	E	284/300 (95%)	250 (88%)	28 (10%)	6 (2%)	7	29
1	F	288/300 (96%)	242 (84%)	38 (13%)	8 (3%)	5	22
1	G	296/300 (99%)	254 (86%)	33 (11%)	9 (3%)	4	20
1	H	294/300 (98%)	243 (83%)	36 (12%)	15 (5%)	2	9
1	I	285/300 (95%)	254 (89%)	28 (10%)	3 (1%)	14	46
1	J	276/300 (92%)	221 (80%)	40 (14%)	15 (5%)	2	9
1	K	268/300 (89%)	221 (82%)	36 (13%)	11 (4%)	3	13
1	L	290/300 (97%)	243 (84%)	37 (13%)	10 (3%)	3	17
All	All	3450/3600 (96%)	2989 (87%)	367 (11%)	94 (3%)	5	23

All (94) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	86	ILE
1	D	38	ALA
1	D	221	ALA
1	E	4	SER
1	E	289	SER
1	F	68	GLY
1	F	87	ASP
1	F	221	ALA
1	G	86	ILE
1	G	143	ARG
1	H	86	ILE
1	H	146	PRO
1	H	148	MET
1	H	221	ALA
1	H	288	ASP
1	H	293	THR
1	I	5	ARG
1	J	3	LEU
1	J	68	GLY
1	J	80	SER
1	J	83	SER
1	J	158	HIS
1	K	26	VAL
1	K	289	SER
1	K	297	ASN
1	L	38	ALA
1	L	141	VAL
1	A	250	GLY
1	A	286	PHE
1	B	40	GLU
1	B	298	ARG
1	C	68	GLY
1	C	226	LYS
1	C	299	LYS
1	D	41	SER
1	E	40	GLU
1	F	86	ILE
1	F	138	LYS
1	H	42	GLU
1	H	227	GLN
1	H	233	GLY
1	H	250	GLY
1	H	265	GLY

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Mol	Chain	Res	Type
1	J	6	ASP
1	J	26	VAL
1	J	37	ASN
1	J	221	ALA
1	J	268	THR
1	K	38	ALA
1	K	225	ASP
1	K	228	GLY
1	L	151	PRO
1	C	298	ARG
1	D	225	ASP
1	E	286	PHE
1	F	40	GLU
1	G	23	ARG
1	G	85	PHE
1	G	144	GLN
1	G	146	PRO
1	H	269	SER
1	H	289	SER
1	J	177	ASP
1	J	226	LYS
1	K	5	ARG
1	K	36	GLY
1	L	192	GLU
1	L	278	PRO
1	A	296	SER
1	D	68	GLY
1	E	69	GLY
1	E	226	LYS
1	F	4	SER
1	J	266	GLY
1	A	37	ASN
1	F	232	THR
1	G	210	LYS
1	H	68	GLY
1	I	6	ASP
1	I	68	GLY
1	J	39	MET
1	L	41	SER
1	L	70	PRO
1	L	83	SER
1	L	251	GLY

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Mol	Chain	Res	Type
1	C	12	ALA
1	G	81	ILE
1	G	68	GLY
1	K	230	VAL
1	L	100	VAL
1	J	233	GLY
1	K	179	ILE
1	K	184	PRO
1	H	220	ILE

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	231/239 (97%)	193 (84%)	38 (16%)	2	9
1	B	233/239 (98%)	200 (86%)	33 (14%)	3	13
1	C	237/239 (99%)	215 (91%)	22 (9%)	9	30
1	D	233/239 (98%)	205 (88%)	28 (12%)	5	19
1	E	225/239 (94%)	188 (84%)	37 (16%)	2	9
1	F	226/239 (95%)	197 (87%)	29 (13%)	4	17
1	G	235/239 (98%)	197 (84%)	38 (16%)	2	10
1	H	234/239 (98%)	201 (86%)	33 (14%)	3	14
1	I	225/239 (94%)	194 (86%)	31 (14%)	3	14
1	J	210/239 (88%)	191 (91%)	19 (9%)	9	32
1	K	188/239 (79%)	164 (87%)	24 (13%)	4	17
1	L	232/239 (97%)	194 (84%)	38 (16%)	2	9
All	All	2709/2868 (94%)	2339 (86%)	370 (14%)	3	15

All (370) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR

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Mol	Chain	Res	Type
1	A	5	ARG
1	A	6	ASP
1	A	7	ASP
1	A	14	VAL
1	A	23	ARG
1	A	24	ARG
1	A	39	MET
1	A	55	MET
1	A	71	GLN
1	A	77	LYS
1	A	79	LEU
1	A	80	SER
1	A	87	ASP
1	A	89	MET
1	A	96	THR
1	A	135	ARG
1	A	142	THR
1	A	187	VAL
1	A	192	GLU
1	A	226	LYS
1	A	232	THR
1	A	236	THR
1	A	239	VAL
1	A	241	GLU
1	A	242	LEU
1	A	243	ILE
1	A	247	THR
1	A	253	LEU
1	A	256	ILE
1	A	278	PRO
1	A	281	VAL
1	A	286	PHE
1	A	289	SER
1	A	291	VAL
1	A	294	LEU
1	A	299	LYS
1	A	300	ARG
1	B	6	ASP
1	B	16	SER
1	B	40	GLU
1	B	41	SER
1	B	54	LEU

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Mol	Chain	Res	Type
1	B	58	VAL
1	B	71	GLN
1	B	76	LEU
1	B	80	SER
1	B	83	SER
1	B	85	PHE
1	B	111	ASP
1	B	115	LEU
1	B	119	HIS
1	B	134	ILE
1	B	139	LEU
1	B	140	THR
1	B	142	THR
1	B	143	ARG
1	B	149	THR
1	B	167	VAL
1	B	187	VAL
1	B	190	ASN
1	B	192	GLU
1	B	219	ASN
1	B	229	GLN
1	B	236	THR
1	B	253	LEU
1	B	255	LYS
1	B	256	ILE
1	B	257	ARG
1	B	282	LEU
1	B	291	VAL
1	C	5	ARG
1	C	6	ASP
1	C	7	ASP
1	C	19	LEU
1	C	24	ARG
1	C	30	LEU
1	C	71	GLN
1	C	138	LYS
1	C	145	THR
1	C	167	VAL
1	C	187	VAL
1	C	223	LEU
1	C	229	GLN
1	C	232	THR

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Mol	Chain	Res	Type
1	C	237	GLU
1	C	245	ASP
1	C	247	THR
1	C	253	LEU
1	C	256	ILE
1	C	258	CYS
1	C	287	THR
1	C	298	ARG
1	D	3	LEU
1	D	4	SER
1	D	5	ARG
1	D	29	THR
1	D	58	VAL
1	D	70	PRO
1	D	83	SER
1	D	107	GLN
1	D	111	ASP
1	D	126	LEU
1	D	143	ARG
1	D	145	THR
1	D	151	PRO
1	D	153	ILE
1	D	167	VAL
1	D	192	GLU
1	D	217	LEU
1	D	219	ASN
1	D	227	GLN
1	D	237	GLU
1	D	243	ILE
1	D	258	CYS
1	D	271	HIS
1	D	287	THR
1	D	291	VAL
1	D	294	LEU
1	D	298	ARG
1	D	299	LYS
1	E	10	GLN
1	E	11	VAL
1	E	14	VAL
1	E	15	LEU
1	E	19	LEU
1	E	24	ARG

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Mol	Chain	Res	Type
1	E	52	VAL
1	E	70	PRO
1	E	72	ILE
1	E	74	ASP
1	E	77	LYS
1	E	92	THR
1	E	93	ASP
1	E	101	GLU
1	E	111	ASP
1	E	142	THR
1	E	153	ILE
1	E	161	GLU
1	E	177	ASP
1	E	189	SER
1	E	190	ASN
1	E	193	SER
1	E	213	LYS
1	E	219	ASN
1	E	237	GLU
1	E	240	ASN
1	E	245	ASP
1	E	253	LEU
1	E	255	LYS
1	E	256	ILE
1	E	258	CYS
1	E	264	GLN
1	E	267	VAL
1	E	287	THR
1	E	288	ASP
1	E	291	VAL
1	E	298	ARG
1	F	13	LYS
1	F	20	PRO
1	F	33	LYS
1	F	37	ASN
1	F	41	SER
1	F	50	ARG
1	F	77	LYS
1	F	82	GLU
1	F	83	SER
1	F	86	ILE
1	F	93	ASP

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Mol	Chain	Res	Type
1	F	113	VAL
1	F	134	ILE
1	F	142	THR
1	F	143	ARG
1	F	154	ILE
1	F	175	LYS
1	F	182	ILE
1	F	193	SER
1	F	219	ASN
1	F	220	ILE
1	F	236	THR
1	F	243	ILE
1	F	253	LEU
1	F	255	LYS
1	F	258	CYS
1	F	281	VAL
1	F	288	ASP
1	F	294	LEU
1	G	29	THR
1	G	30	LEU
1	G	41	SER
1	G	42	GLU
1	G	43	GLU
1	G	58	VAL
1	G	60	ILE
1	G	71	GLN
1	G	72	ILE
1	G	83	SER
1	G	85	PHE
1	G	86	ILE
1	G	90	ARG
1	G	102	MET
1	G	118	ARG
1	G	126	LEU
1	G	142	THR
1	G	143	ARG
1	G	144	GLN
1	G	146	PRO
1	G	147	GLU
1	G	151	PRO
1	G	152	GLU
1	G	153	ILE

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Mol	Chain	Res	Type
1	G	161	GLU
1	G	172	MET
1	G	189	SER
1	G	192	GLU
1	G	199	ASP
1	G	212	GLU
1	G	220	ILE
1	G	258	CYS
1	G	260	LEU
1	G	269	SER
1	G	271	HIS
1	G	272	ILE
1	G	273	ILE
1	G	294	LEU
1	H	3	LEU
1	H	10	GLN
1	H	13	LYS
1	H	14	VAL
1	H	16	SER
1	H	17	GLU
1	H	37	ASN
1	H	39	MET
1	H	43	GLU
1	H	54	LEU
1	H	82	GLU
1	H	97	MET
1	H	107	GLN
1	H	132	GLU
1	H	143	ARG
1	H	144	GLN
1	H	146	PRO
1	H	147	GLU
1	H	175	LYS
1	H	187	VAL
1	H	215	MET
1	H	220	ILE
1	H	231	LEU
1	H	234	LEU
1	H	235	SER
1	H	243	ILE
1	H	249	TYR
1	H	258	CYS

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Mol	Chain	Res	Type
1	H	267	VAL
1	H	268	THR
1	H	271	HIS
1	H	288	ASP
1	H	289	SER
1	I	3	LEU
1	I	6	ASP
1	I	7	ASP
1	I	10	GLN
1	I	19	LEU
1	I	26	VAL
1	I	44	LEU
1	I	78	ARG
1	I	80	SER
1	I	82	GLU
1	I	86	ILE
1	I	87	ASP
1	I	89	MET
1	I	92	THR
1	I	99	VAL
1	I	103	VAL
1	I	111	ASP
1	I	118	ARG
1	I	129	LYS
1	I	139	LEU
1	I	155	ASP
1	I	167	VAL
1	I	177	ASP
1	I	192	GLU
1	I	223	LEU
1	I	224	MET
1	I	232	THR
1	I	235	SER
1	I	237	GLU
1	I	255	LYS
1	I	271	HIS
1	J	5	ARG
1	J	28	LYS
1	J	37	ASN
1	J	40	GLU
1	J	52	VAL
1	J	70	PRO

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Mol	Chain	Res	Type
1	J	72	ILE
1	J	80	SER
1	J	101	GLU
1	J	118	ARG
1	J	171	ASN
1	J	192	GLU
1	J	195	ASN
1	J	219	ASN
1	J	226	LYS
1	J	249	TYR
1	J	269	SER
1	J	294	LEU
1	J	296	SER
1	K	13	LYS
1	K	16	SER
1	K	23	ARG
1	K	41	SER
1	K	58	VAL
1	K	80	SER
1	K	82	GLU
1	K	83	SER
1	K	109	ASN
1	K	124	ILE
1	K	126	LEU
1	K	129	LYS
1	K	166	ASN
1	K	172	MET
1	K	177	ASP
1	K	197	ASN
1	K	199	ASP
1	K	200	LEU
1	K	231	LEU
1	K	252	MET
1	K	256	ILE
1	K	269	SER
1	K	281	VAL
1	K	297	ASN
1	L	4	SER
1	L	5	ARG
1	L	6	ASP
1	L	17	GLU
1	L	24	ARG

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Mol	Chain	Res	Type
1	L	26	VAL
1	L	33	LYS
1	L	39	MET
1	L	41	SER
1	L	55	MET
1	L	78	ARG
1	L	85	PHE
1	L	87	ASP
1	L	99	VAL
1	L	108	VAL
1	L	124	ILE
1	L	143	ARG
1	L	155	ASP
1	L	156	ILE
1	L	172	MET
1	L	177	ASP
1	L	192	GLU
1	L	193	SER
1	L	197	ASN
1	L	213	LYS
1	L	227	GLN
1	L	229	GLN
1	L	240	ASN
1	L	241	GLU
1	L	245	ASP
1	L	252	MET
1	L	256	ILE
1	L	258	CYS
1	L	278	PRO
1	L	287	THR
1	L	291	VAL
1	L	296	SER
1	L	297	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (64) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	37	ASN
1	A	84	HIS
1	A	117	ASN
1	A	238	GLN

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Mol	Chain	Res	Type
1	A	240	ASN
1	B	71	GLN
1	B	107	GLN
1	B	109	ASN
1	B	119	HIS
1	B	171	ASN
1	B	219	ASN
1	B	229	GLN
1	B	238	GLN
1	B	240	ASN
1	B	279	ASN
1	C	107	GLN
1	C	238	GLN
1	C	264	GLN
1	D	119	HIS
1	D	219	ASN
1	D	229	GLN
1	E	117	ASN
1	E	171	ASN
1	E	238	GLN
1	F	37	ASN
1	F	84	HIS
1	F	171	ASN
1	F	219	ASN
1	F	240	ASN
1	G	119	HIS
1	G	195	ASN
1	G	227	GLN
1	G	240	ASN
1	G	297	ASN
1	H	10	GLN
1	H	37	ASN
1	H	107	GLN
1	H	195	ASN
1	H	271	HIS
1	I	107	GLN
1	I	117	ASN
1	I	271	HIS
1	J	195	ASN
1	J	219	ASN
1	J	240	ASN
1	J	264	GLN

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Mol	Chain	Res	Type
1	J	297	ASN
1	K	107	GLN
1	K	109	ASN
1	K	114	ASN
1	K	166	ASN
1	K	190	ASN
1	K	197	ASN
1	K	297	ASN
1	L	84	HIS
1	L	114	ASN
1	L	117	ASN
1	L	195	ASN
1	L	197	ASN
1	L	227	GLN
1	L	229	GLN
1	L	240	ASN
1	L	279	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 34 ligands modelled in this entry, 14 are monoatomic - leaving 20 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	1300	4	24,29,29	1.97	5 (20%)	29,45,45	2.08	5 (17%)
2	NLG	B	1302	-	6,12,12	5.37	3 (50%)	7,15,15	7.19	5 (71%)
2	NLG	G	1301	-	6,12,12	5.14	3 (50%)	7,15,15	6.00	4 (57%)
3	ADP	J	1298	-	24,29,29	2.66	8 (33%)	29,45,45	2.24	9 (31%)
3	ADP	L	1300	4	24,29,29	1.98	5 (20%)	29,45,45	2.07	6 (20%)
3	ADP	E	1299	4	24,29,29	2.05	6 (25%)	29,45,45	2.08	6 (20%)
2	NLG	K	1298	-	6,12,12	5.13	4 (66%)	7,15,15	6.22	4 (57%)
3	ADP	G	1299	4	24,29,29	1.86	5 (20%)	29,45,45	2.04	7 (24%)
2	NLG	E	1301	-	6,12,12	5.19	3 (50%)	7,15,15	6.90	5 (71%)
2	NLG	D	1302	-	6,12,12	5.15	3 (50%)	7,15,15	6.53	4 (57%)
3	ADP	F	1299	-	24,29,29	1.93	4 (16%)	29,45,45	2.04	5 (17%)
2	NLG	I	1300	-	6,12,12	5.16	3 (50%)	7,15,15	6.83	4 (57%)
3	ADP	C	1300	4	24,29,29	2.00	5 (20%)	29,45,45	2.20	6 (20%)
2	NLG	L	1302	-	6,12,12	5.18	3 (50%)	7,15,15	6.75	5 (71%)
2	NLG	A	1302	-	6,12,12	5.20	3 (50%)	7,15,15	6.80	5 (71%)
3	ADP	I	1298	4	24,29,29	1.79	4 (16%)	29,45,45	1.95	6 (20%)
2	NLG	F	1300	-	6,12,12	5.13	3 (50%)	7,15,15	6.90	4 (57%)
3	ADP	H	1297	4	24,29,29	1.91	6 (25%)	29,45,45	2.11	8 (27%)
3	ADP	D	1300	4	24,29,29	1.82	3 (12%)	29,45,45	2.00	6 (20%)
2	NLG	H	1299	-	6,12,12	5.40	3 (50%)	7,15,15	6.44	5 (71%)

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	1300	4	-	2/12/32/32	0/3/3/3
2	NLG	B	1302	-	-	0/7/13/13	-
2	NLG	G	1301	-	-	2/7/13/13	-
3	ADP	J	1298	-	-	2/12/32/32	0/3/3/3
3	ADP	L	1300	4	-	3/12/32/32	0/3/3/3
3	ADP	E	1299	4	-	1/12/32/32	0/3/3/3
2	NLG	K	1298	-	-	2/7/13/13	-
3	ADP	G	1299	4	-	1/12/32/32	0/3/3/3
2	NLG	E	1301	-	-	0/7/13/13	-
2	NLG	D	1302	-	-	1/7/13/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	F	1299	-	-	1/12/32/32	0/3/3/3
2	NLG	I	1300	-	-	1/7/13/13	-
3	ADP	C	1300	4	-	2/12/32/32	0/3/3/3
2	NLG	L	1302	-	-	1/7/13/13	-
2	NLG	A	1302	-	-	0/7/13/13	-
3	ADP	I	1298	4	-	1/12/32/32	0/3/3/3
2	NLG	F	1300	-	-	1/7/13/13	-
3	ADP	H	1297	4	-	4/12/32/32	0/3/3/3
3	ADP	D	1300	4	-	4/12/32/32	0/3/3/3
2	NLG	H	1299	-	-	1/7/13/13	-

All (82) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	1299	NLG	C8-C7	-10.23	1.29	1.50
2	G	1301	NLG	C8-C7	-10.02	1.29	1.50
2	B	1302	NLG	C8-C7	-9.63	1.30	1.50
2	D	1302	NLG	C8-C7	-9.61	1.30	1.50
2	K	1298	NLG	C8-C7	-9.57	1.30	1.50
2	E	1301	NLG	C8-C7	-9.45	1.30	1.50
2	F	1300	NLG	C8-C7	-9.38	1.31	1.50
2	A	1302	NLG	C8-C7	-9.36	1.31	1.50
2	I	1300	NLG	C8-C7	-9.34	1.31	1.50
2	L	1302	NLG	C8-C7	-9.28	1.31	1.50
3	E	1299	ADP	C4-N3	6.62	1.44	1.35
2	D	1302	NLG	C7-N2	-6.39	1.12	1.34
2	E	1301	NLG	C7-N2	-6.37	1.12	1.34
2	H	1299	NLG	C7-N2	-6.37	1.12	1.34
3	J	1298	ADP	C4-N3	6.36	1.44	1.35
2	B	1302	NLG	CA-N2	6.33	1.54	1.46
2	A	1302	NLG	C7-N2	-6.26	1.12	1.34
3	B	1300	ADP	C4-N3	6.13	1.44	1.35
2	F	1300	NLG	C7-N2	-6.04	1.13	1.34
3	D	1300	ADP	C4-N3	6.03	1.44	1.35
3	F	1299	ADP	C4-N3	6.01	1.43	1.35
3	L	1300	ADP	C4-N3	6.01	1.43	1.35
3	J	1298	ADP	O4'-C1'	6.00	1.49	1.41
3	C	1300	ADP	C4-N3	5.97	1.43	1.35
2	L	1302	NLG	C7-N2	-5.94	1.14	1.34
2	B	1302	NLG	C7-N2	-5.91	1.14	1.34
2	G	1301	NLG	C7-N2	-5.90	1.14	1.34
2	I	1300	NLG	C7-N2	-5.85	1.14	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	1300	NLG	CA-N2	5.84	1.54	1.46
3	H	1297	ADP	C4-N3	5.82	1.43	1.35
2	L	1302	NLG	CA-N2	5.79	1.54	1.46
2	K	1298	NLG	C7-N2	-5.61	1.15	1.34
2	A	1302	NLG	CA-N2	5.60	1.53	1.46
3	I	1298	ADP	C4-N3	5.40	1.43	1.35
2	F	1300	NLG	CA-N2	5.33	1.53	1.46
2	E	1301	NLG	CA-N2	5.19	1.53	1.46
3	G	1299	ADP	C4-N3	5.17	1.42	1.35
2	H	1299	NLG	CA-N2	5.05	1.53	1.46
2	K	1298	NLG	CA-N2	4.70	1.52	1.46
2	D	1302	NLG	CA-N2	4.61	1.52	1.46
3	J	1298	ADP	C3'-C4'	-4.25	1.42	1.53
2	G	1301	NLG	CA-N2	4.13	1.52	1.46
3	J	1298	ADP	O3'-C3'	4.04	1.52	1.43
3	F	1299	ADP	C2-N1	4.00	1.41	1.33
3	E	1299	ADP	C2-N1	3.99	1.41	1.33
3	B	1300	ADP	C2-N1	3.93	1.41	1.33
3	L	1300	ADP	C2-N1	3.87	1.41	1.33
3	C	1300	ADP	C2-N1	3.86	1.41	1.33
3	H	1297	ADP	C2-N1	3.78	1.40	1.33
3	D	1300	ADP	C2-N1	3.70	1.40	1.33
3	J	1298	ADP	C2'-C1'	-3.69	1.48	1.53
3	G	1299	ADP	C2-N1	3.67	1.40	1.33
3	L	1300	ADP	C8-N7	-3.64	1.28	1.34
3	I	1298	ADP	C2-N1	3.58	1.40	1.33
3	D	1300	ADP	C8-N7	-3.55	1.28	1.34
3	G	1299	ADP	C8-N7	-3.55	1.28	1.34
3	J	1298	ADP	C2-N1	3.52	1.40	1.33
3	E	1299	ADP	C8-N7	-3.43	1.28	1.34
3	F	1299	ADP	C8-N7	-3.42	1.28	1.34
3	I	1298	ADP	C8-N7	-3.24	1.28	1.34
3	B	1300	ADP	C8-N7	-3.15	1.29	1.34
3	H	1297	ADP	C8-N7	-3.13	1.29	1.34
3	C	1300	ADP	C8-N7	-3.08	1.29	1.34
2	K	1298	NLG	CB-CA	-3.07	1.49	1.53
3	C	1300	ADP	O4'-C1'	2.98	1.45	1.41
3	E	1299	ADP	O3'-C3'	2.54	1.49	1.43
3	H	1297	ADP	O4'-C1'	2.46	1.44	1.41
3	B	1300	ADP	O3'-C3'	2.45	1.48	1.43
3	J	1298	ADP	C8-N7	-2.44	1.30	1.34
3	L	1300	ADP	PA-O2A	-2.44	1.43	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	1298	ADP	C2'-C3'	2.40	1.59	1.53
3	G	1299	ADP	O4'-C1'	2.39	1.44	1.41
3	E	1299	ADP	C2-N3	2.27	1.35	1.32
3	H	1297	ADP	PA-O2A	-2.20	1.45	1.55
3	H	1297	ADP	O3'-C3'	2.17	1.48	1.43
3	C	1300	ADP	O3'-C3'	2.14	1.48	1.43
3	L	1300	ADP	C2-N3	2.12	1.35	1.32
3	F	1299	ADP	PA-O2A	-2.11	1.45	1.55
3	I	1298	ADP	PA-O2A	-2.07	1.45	1.55
3	B	1300	ADP	PA-O2A	-2.05	1.45	1.55
3	E	1299	ADP	PA-O2A	-2.04	1.45	1.55
3	G	1299	ADP	PA-O2A	-2.01	1.45	1.55

All (109) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1302	NLG	CA-N2-C7	16.77	140.87	122.44
2	F	1300	NLG	CA-N2-C7	15.85	139.86	122.44
2	E	1301	NLG	CA-N2-C7	15.77	139.77	122.44
2	A	1302	NLG	CA-N2-C7	15.44	139.41	122.44
2	I	1300	NLG	CA-N2-C7	15.26	139.22	122.44
2	L	1302	NLG	CA-N2-C7	14.95	138.87	122.44
2	D	1302	NLG	CA-N2-C7	14.49	138.36	122.44
2	H	1299	NLG	CA-N2-C7	14.27	138.12	122.44
2	G	1301	NLG	CA-N2-C7	11.71	135.31	122.44
2	K	1298	NLG	CA-N2-C7	11.53	135.11	122.44
2	K	1298	NLG	CB-CG-CD	-7.45	97.57	113.59
2	K	1298	NLG	C8-C7-N2	7.16	128.22	116.10
3	C	1300	ADP	C5-C6-N6	7.06	131.09	120.35
2	G	1301	NLG	C8-C7-N2	6.96	127.88	116.10
3	J	1298	ADP	C5-C6-N6	6.94	130.90	120.35
3	D	1300	ADP	C5-C6-N6	6.82	130.71	120.35
2	L	1302	NLG	C8-C7-N2	6.74	127.52	116.10
3	F	1299	ADP	C5-C6-N6	6.70	130.54	120.35
2	A	1302	NLG	C8-C7-N2	6.70	127.44	116.10
2	I	1300	NLG	C8-C7-N2	6.69	127.42	116.10
3	H	1297	ADP	C5-C6-N6	6.66	130.47	120.35
2	E	1301	NLG	C8-C7-N2	6.64	127.35	116.10
3	I	1298	ADP	C5-C6-N6	6.62	130.41	120.35
2	H	1299	NLG	C8-C7-N2	6.53	127.16	116.10
2	D	1302	NLG	C8-C7-N2	6.51	127.12	116.10
3	G	1299	ADP	C5-C6-N6	6.43	130.12	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1300	NLG	C8-C7-N2	6.42	126.97	116.10
3	B	1300	ADP	C5-C6-N6	6.42	130.10	120.35
2	B	1302	NLG	C8-C7-N2	6.41	126.96	116.10
3	L	1300	ADP	C5-C6-N6	6.28	129.90	120.35
2	G	1301	NLG	CB-CG-CD	-6.22	100.22	113.59
3	E	1299	ADP	C5-C6-N6	6.17	129.72	120.35
3	E	1299	ADP	C1'-N9-C4	5.74	136.72	126.64
3	L	1300	ADP	C1'-N9-C4	5.39	136.12	126.64
2	E	1301	NLG	O7-C7-N2	-5.13	112.53	121.95
2	D	1302	NLG	O7-C7-N2	-5.10	112.57	121.95
2	A	1302	NLG	O7-C7-N2	-5.07	112.62	121.95
3	C	1300	ADP	C1'-N9-C4	5.05	135.52	126.64
2	K	1298	NLG	O7-C7-N2	-5.04	112.69	121.95
2	G	1301	NLG	O7-C7-N2	-5.01	112.74	121.95
2	L	1302	NLG	O7-C7-N2	-5.00	112.76	121.95
3	F	1299	ADP	C1'-N9-C4	4.96	135.35	126.64
2	I	1300	NLG	O7-C7-N2	-4.93	112.89	121.95
2	H	1299	NLG	O7-C7-N2	-4.88	112.98	121.95
3	G	1299	ADP	C1'-N9-C4	4.82	135.12	126.64
3	H	1297	ADP	C1'-N9-C4	4.81	135.10	126.64
2	F	1300	NLG	O7-C7-N2	-4.75	113.21	121.95
3	B	1300	ADP	C1'-N9-C4	4.72	134.94	126.64
3	J	1298	ADP	O5'-C5'-C4'	4.63	124.93	108.99
2	B	1302	NLG	O7-C7-N2	-4.58	113.53	121.95
2	I	1300	NLG	CB-CG-CD	-4.37	104.20	113.59
2	D	1302	NLG	CB-CG-CD	-4.33	104.28	113.59
3	I	1298	ADP	C1'-N9-C4	4.16	133.96	126.64
2	L	1302	NLG	CB-CG-CD	-3.93	105.14	113.59
2	H	1299	NLG	CB-CG-CD	-3.62	105.82	113.59
2	F	1300	NLG	CB-CG-CD	-3.57	105.91	113.59
3	C	1300	ADP	C3'-C2'-C1'	3.55	106.32	100.98
3	B	1300	ADP	C4-C5-N7	3.54	113.09	109.40
3	J	1298	ADP	C1'-N9-C4	3.51	132.80	126.64
3	D	1300	ADP	C1'-N9-C4	3.48	132.75	126.64
3	E	1299	ADP	C4-C5-N7	3.46	113.01	109.40
3	J	1298	ADP	N6-C6-N1	-3.39	111.53	118.57
3	L	1300	ADP	C4-C5-N7	3.38	112.92	109.40
3	G	1299	ADP	C4-C5-N7	3.32	112.86	109.40
3	D	1300	ADP	N6-C6-N1	-3.26	111.81	118.57
3	L	1300	ADP	C3'-C2'-C1'	3.23	105.85	100.98
3	C	1300	ADP	N6-C6-N1	-3.18	111.97	118.57
3	I	1298	ADP	N6-C6-N1	-3.18	111.98	118.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1300	ADP	C3'-C2'-C1'	3.14	105.71	100.98
3	I	1298	ADP	C3'-C2'-C1'	3.11	105.67	100.98
3	F	1299	ADP	C3'-C2'-C1'	3.11	105.66	100.98
3	F	1299	ADP	C4-C5-N7	3.08	112.61	109.40
3	D	1300	ADP	C3'-C2'-C1'	3.08	105.61	100.98
3	H	1297	ADP	C4-C5-N7	3.06	112.59	109.40
3	E	1299	ADP	C3'-C2'-C1'	3.05	105.58	100.98
3	H	1297	ADP	N6-C6-N1	-2.99	112.38	118.57
3	F	1299	ADP	N6-C6-N1	-2.96	112.43	118.57
3	I	1298	ADP	C4-C5-N7	2.93	112.45	109.40
3	J	1298	ADP	C4-C5-N7	2.90	112.42	109.40
2	B	1302	NLG	CB-CG-CD	-2.88	107.40	113.59
2	E	1301	NLG	CB-CA-N2	2.87	114.37	110.19
3	C	1300	ADP	C4-C5-N7	2.84	112.36	109.40
2	B	1302	NLG	CB-CA-N2	2.82	114.30	110.19
3	L	1300	ADP	N6-C6-N1	-2.79	112.78	118.57
3	D	1300	ADP	C4-C5-N7	2.76	112.27	109.40
3	E	1299	ADP	N6-C6-N1	-2.74	112.88	118.57
3	B	1300	ADP	N6-C6-N1	-2.74	112.89	118.57
3	C	1300	ADP	O5'-C5'-C4'	2.74	118.41	108.99
2	L	1302	NLG	CB-CA-N2	2.72	114.16	110.19
3	G	1299	ADP	C3'-C2'-C1'	2.71	105.05	100.98
3	G	1299	ADP	N6-C6-N1	-2.70	112.97	118.57
3	J	1298	ADP	O4'-C4'-C5'	2.70	118.25	109.37
3	E	1299	ADP	O3'-C3'-C4'	-2.64	103.40	111.05
3	H	1297	ADP	O3'-C3'-C4'	-2.62	103.48	111.05
3	J	1298	ADP	C2'-C3'-C4'	2.61	107.71	102.64
3	J	1298	ADP	O4'-C4'-C3'	-2.60	99.96	105.11
2	A	1302	NLG	CB-CA-N2	2.59	113.97	110.19
3	I	1298	ADP	O3'-C3'-C4'	-2.59	103.56	111.05
2	A	1302	NLG	CB-CG-CD	-2.44	108.34	113.59
3	H	1297	ADP	C3'-C2'-C1'	2.41	104.60	100.98
3	L	1300	ADP	O3'-C3'-C4'	-2.39	104.13	111.05
3	H	1297	ADP	O4'-C4'-C3'	-2.38	100.40	105.11
3	D	1300	ADP	O3'-C3'-C4'	-2.31	104.38	111.05
3	G	1299	ADP	O4'-C4'-C3'	-2.23	100.70	105.11
2	H	1299	NLG	CB-CA-N2	2.20	113.41	110.19
3	H	1297	ADP	PA-O3A-PB	2.18	140.30	132.83
2	E	1301	NLG	CB-CG-CD	-2.15	108.96	113.59
3	G	1299	ADP	O5'-C5'-C4'	2.03	115.97	108.99
3	J	1298	ADP	PA-O3A-PB	2.01	139.73	132.83

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	K	1298	NLG	CA-CB-CG-CD
3	B	1300	ADP	PA-O3A-PB-O3B
3	J	1298	ADP	PA-O3A-PB-O3B
3	J	1298	ADP	C4'-C5'-O5'-PA
3	C	1300	ADP	C4'-C5'-O5'-PA
2	H	1299	NLG	CA-CB-CG-CD
2	D	1302	NLG	CA-CB-CG-CD
2	K	1298	NLG	C-CA-N2-C7
2	L	1302	NLG	CA-CB-CG-CD
2	I	1300	NLG	CA-CB-CG-CD
3	D	1300	ADP	C4'-C5'-O5'-PA
2	G	1301	NLG	CA-CB-CG-CD
3	F	1299	ADP	C4'-C5'-O5'-PA
3	E	1299	ADP	C4'-C5'-O5'-PA
3	I	1298	ADP	C4'-C5'-O5'-PA
3	C	1300	ADP	PA-O3A-PB-O1B
3	H	1297	ADP	C4'-C5'-O5'-PA
3	G	1299	ADP	C4'-C5'-O5'-PA
3	B	1300	ADP	C4'-C5'-O5'-PA
3	L	1300	ADP	C4'-C5'-O5'-PA
3	D	1300	ADP	PA-O3A-PB-O1B
2	F	1300	NLG	CA-CB-CG-CD
3	L	1300	ADP	PA-O3A-PB-O2B
3	L	1300	ADP	PA-O3A-PB-O3B
3	H	1297	ADP	PA-O3A-PB-O2B
3	H	1297	ADP	PA-O3A-PB-O3B
3	D	1300	ADP	PA-O3A-PB-O2B
3	D	1300	ADP	PA-O3A-PB-O3B
3	H	1297	ADP	PA-O3A-PB-O1B
2	G	1301	NLG	C-CA-N2-C7

There are no ring outliers.

15 monomers are involved in 53 short contacts:

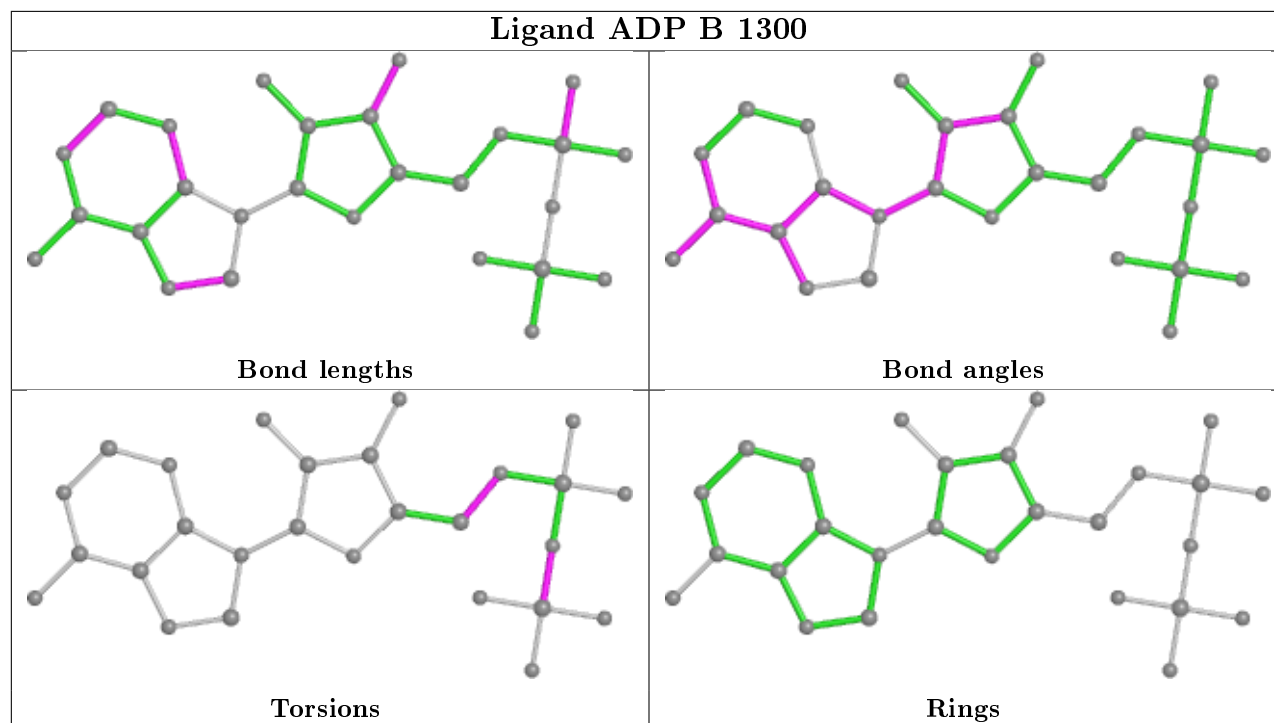
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1300	ADP	2	0
2	G	1301	NLG	4	0
3	J	1298	ADP	13	0
3	L	1300	ADP	3	0
3	E	1299	ADP	3	0
2	K	1298	NLG	4	0

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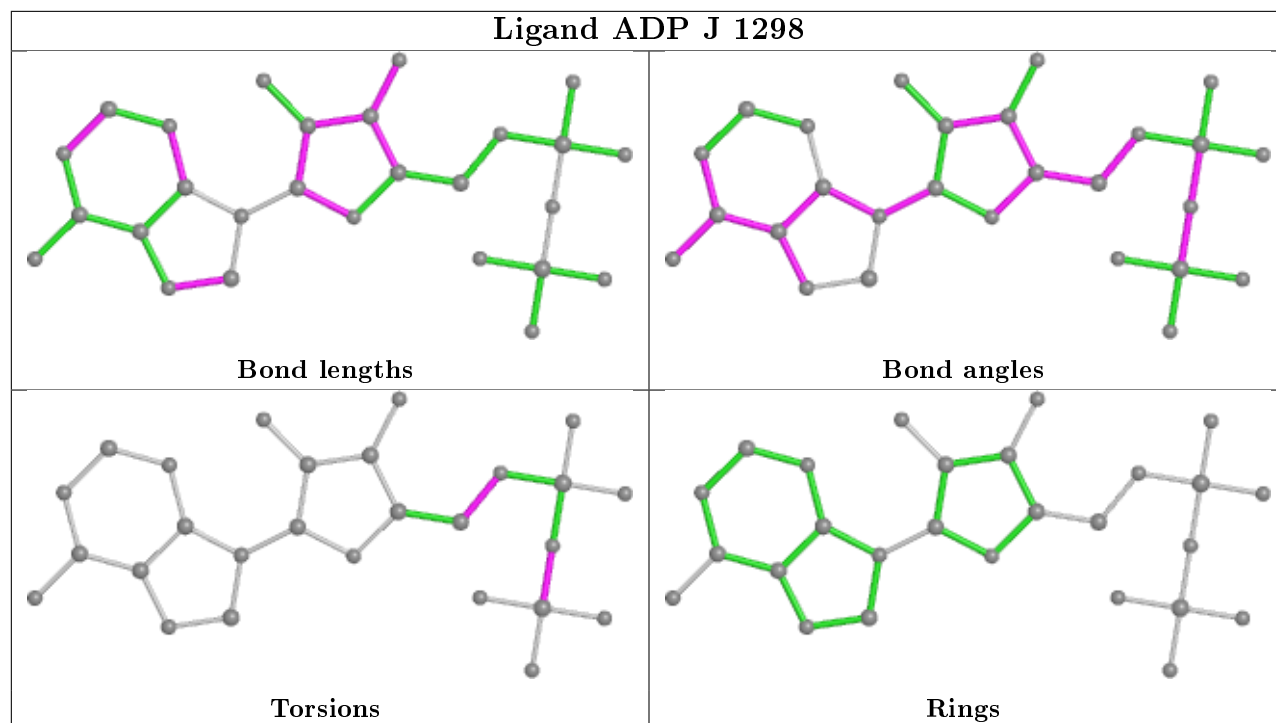
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	1299	ADP	1	0
2	D	1302	NLG	1	0
3	F	1299	ADP	2	0
2	I	1300	NLG	1	0
3	C	1300	ADP	2	0
2	L	1302	NLG	3	0
2	F	1300	NLG	3	0
3	H	1297	ADP	5	0
2	H	1299	NLG	6	0

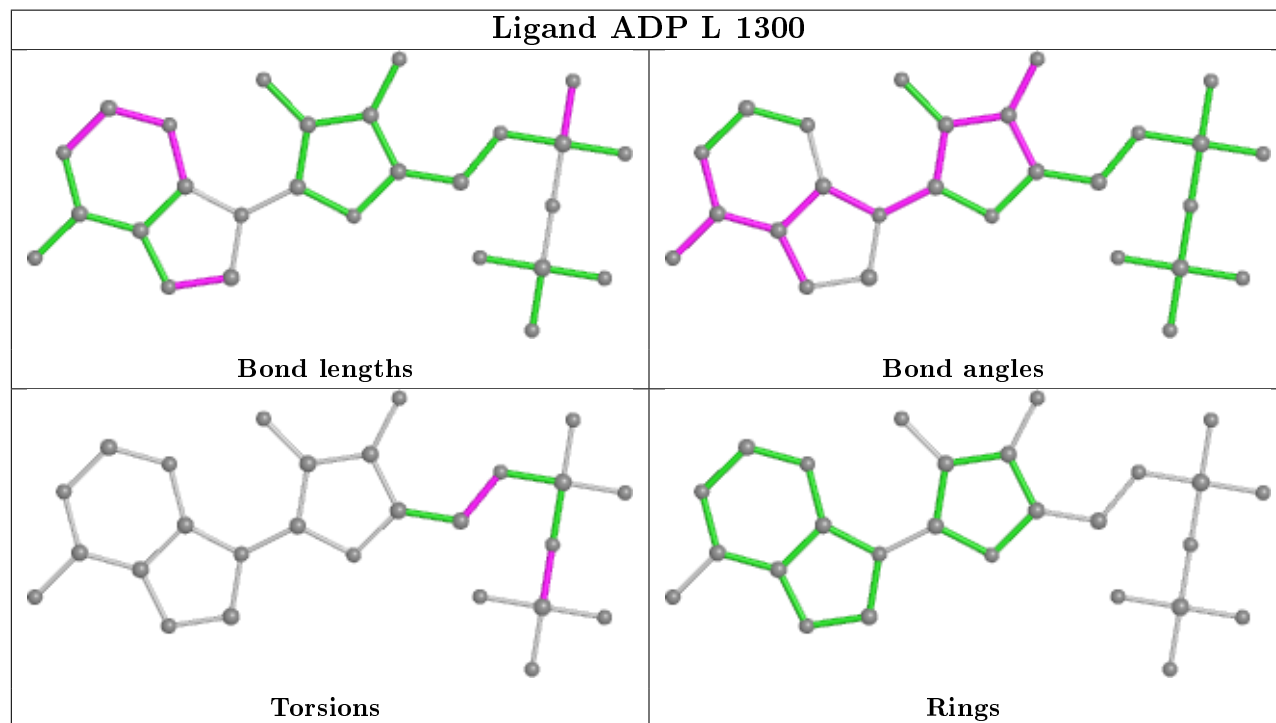
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



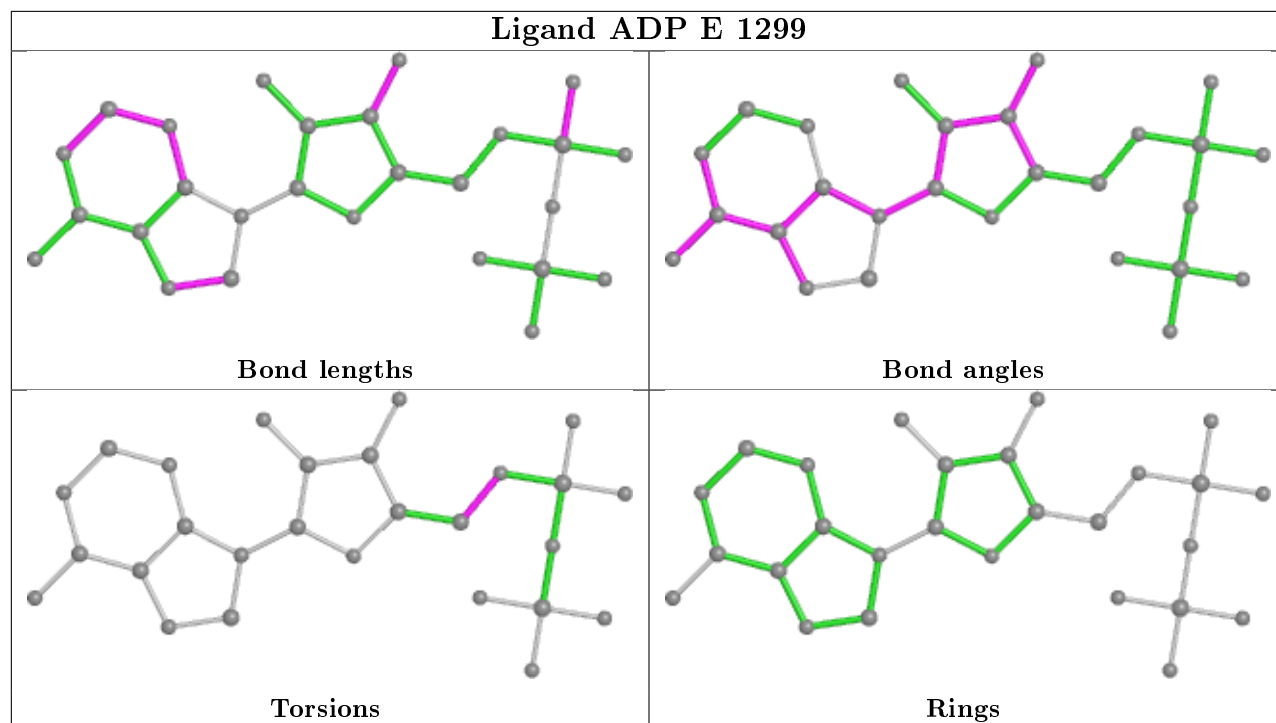
## Ligand ADP J 1298



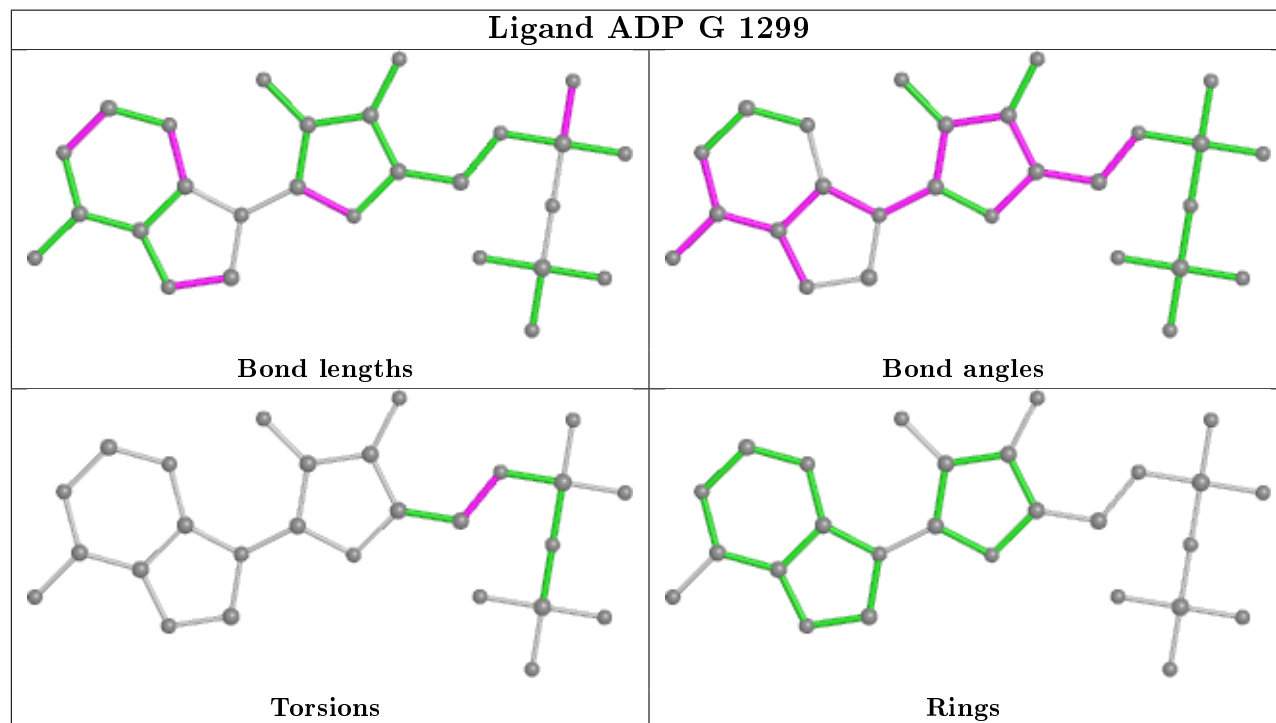
## Ligand ADP L 1300



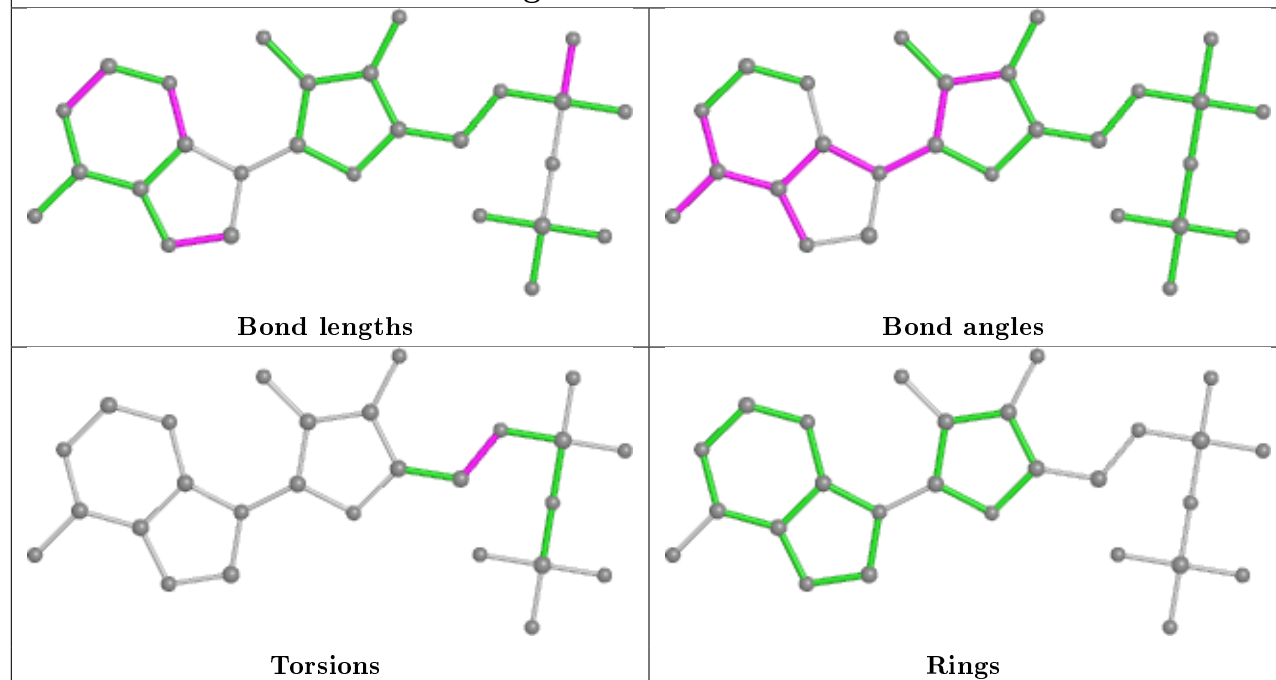
## Ligand ADP E 1299



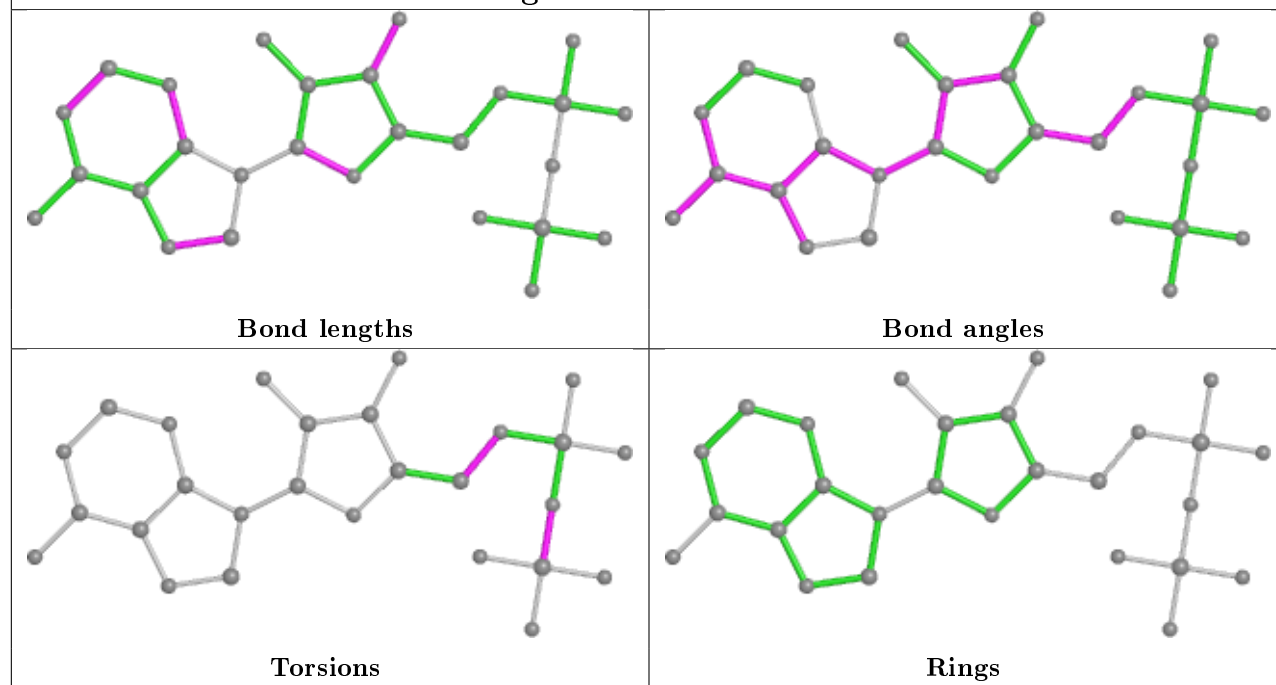
## Ligand ADP G 1299



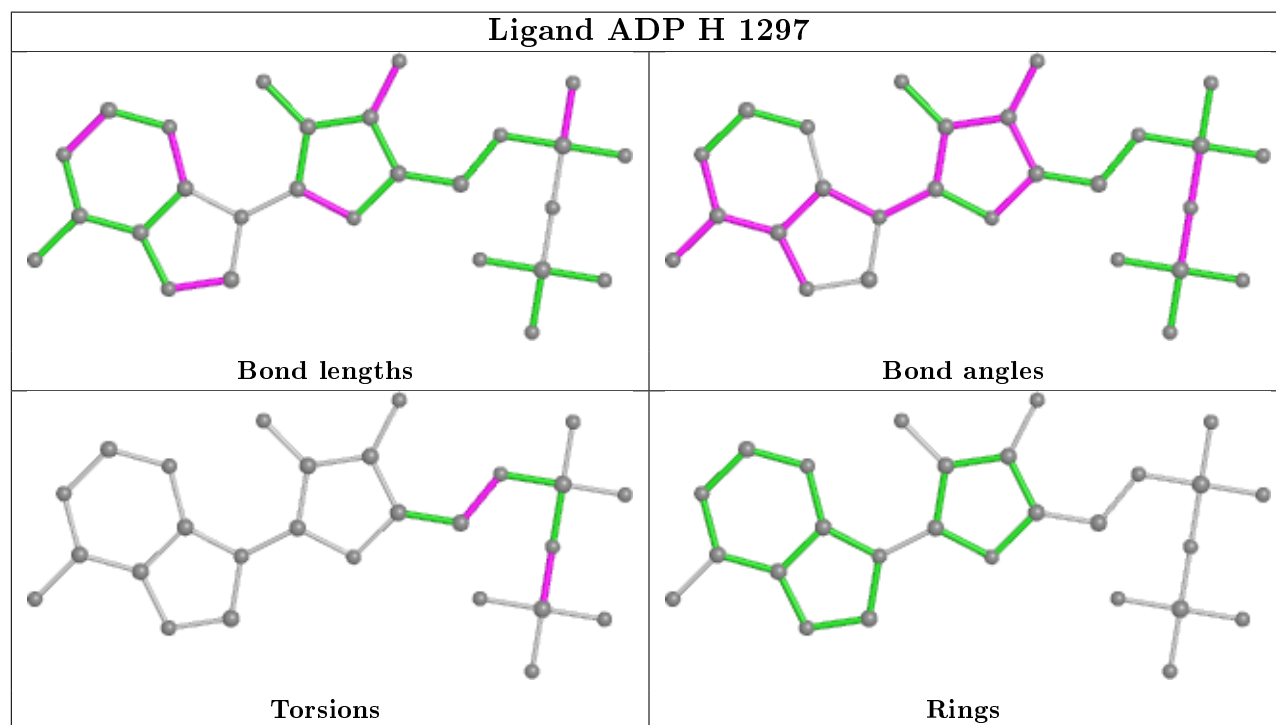
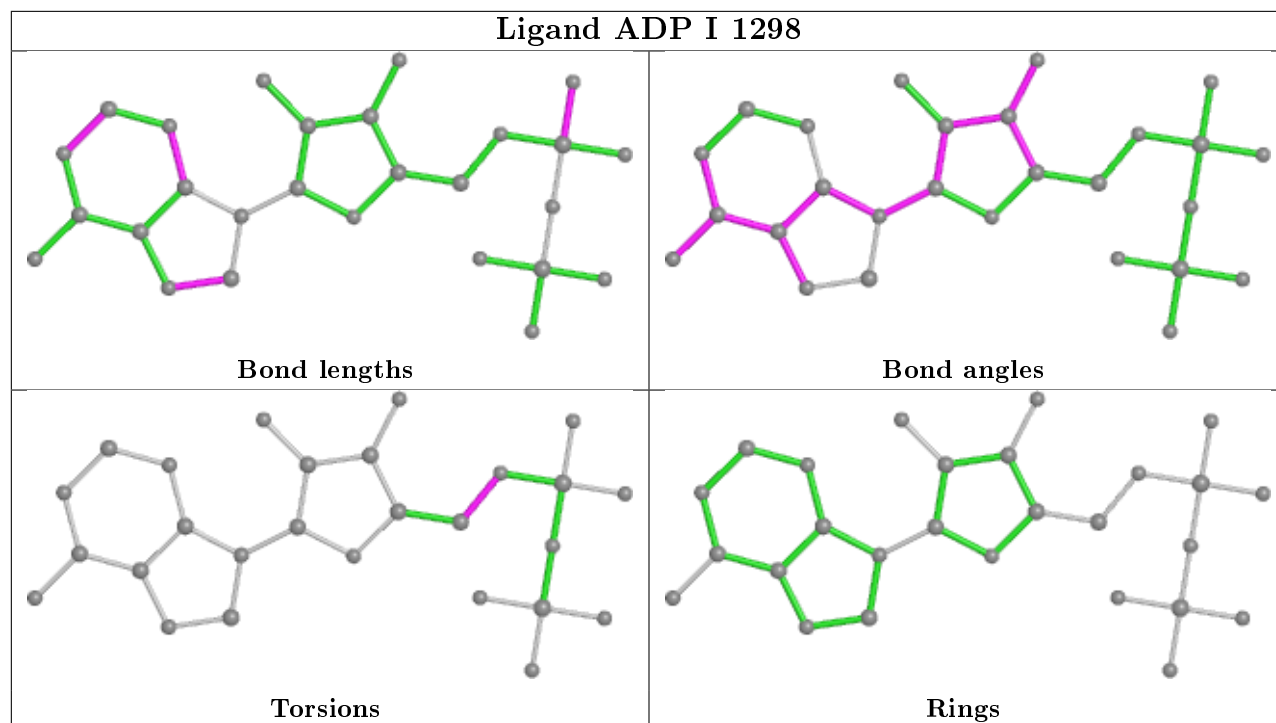
## Ligand ADP F 1299

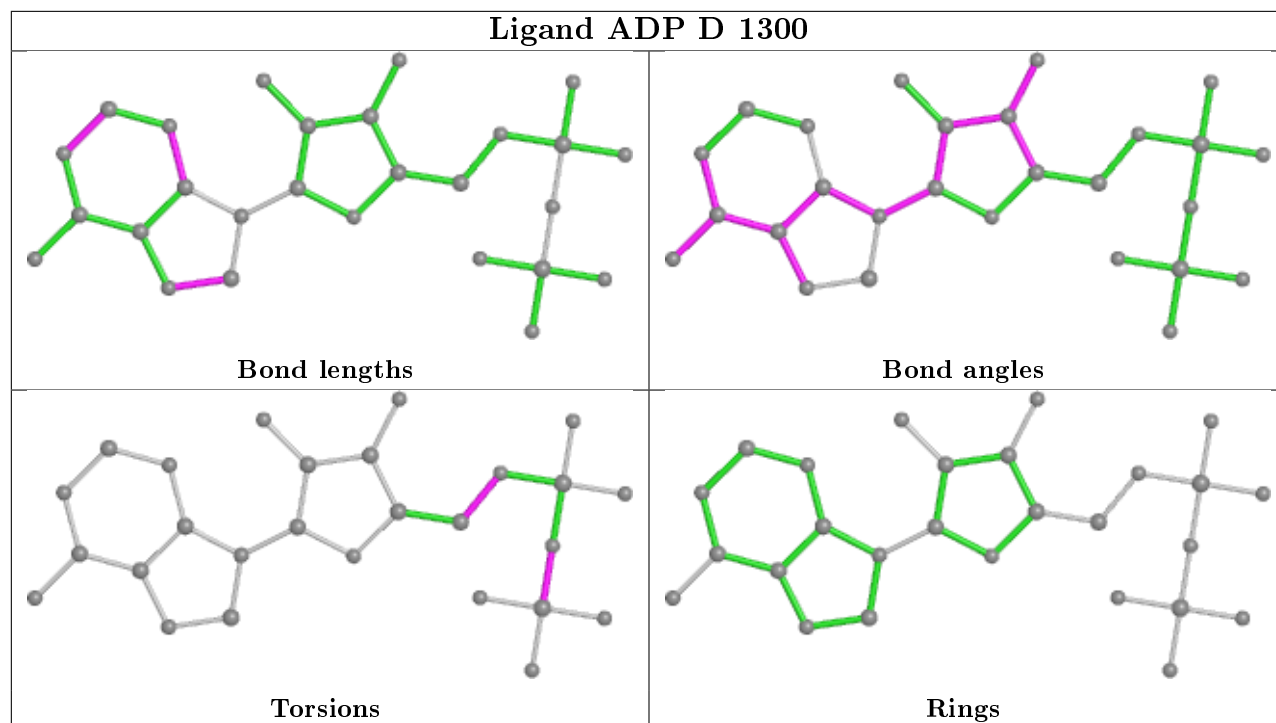


## Ligand ADP C 1300









## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q < 0.9
1	A	292/300 (97%)	0.29	8 (2%) 54 38	28, 67, 120, 133	0
1	B	297/300 (99%)	0.27	8 (2%) 54 38	31, 63, 103, 130	0
1	C	299/300 (99%)	0.16	1 (0%) 94 87	21, 47, 92, 115	0
1	D	295/300 (98%)	0.20	1 (0%) 94 87	17, 46, 88, 132	0
1	E	288/300 (96%)	0.44	16 (5%) 24 15	52, 82, 128, 158	0
1	F	292/300 (97%)	0.54	22 (7%) 14 8	45, 90, 139, 157	0
1	G	298/300 (99%)	0.54	25 (8%) 11 6	49, 87, 124, 155	0
1	H	296/300 (98%)	0.74	36 (12%) 4 2	53, 106, 135, 142	0
1	I	289/300 (96%)	0.45	14 (4%) 30 19	45, 84, 123, 147	0
1	J	280/300 (93%)	1.28	74 (26%) 0 0	80, 126, 157, 164	0
1	K	274/300 (91%)	1.93	108 (39%) 0 0	106, 140, 161, 167	0
1	L	294/300 (98%)	0.82	33 (11%) 5 3	69, 102, 131, 151	0
All	All	3494/3600 (97%)	0.63	346 (9%) 7 4	17, 85, 147, 167	0

All (346) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	2	THR	10.4
1	K	293	THR	10.3
1	K	3	LEU	10.2
1	K	213	LYS	9.7
1	K	68	GLY	8.7
1	J	15	LEU	8.2
1	H	286	PHE	8.2
1	I	2	THR	7.9
1	H	37	ASN	7.7
1	J	220	ILE	7.6
1	K	247	THR	7.3

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Mol	Chain	Res	Type	RSRZ
1	K	296	SER	7.2
1	K	285	ILE	7.0
1	K	67	GLY	6.7
1	G	2	THR	6.6
1	K	231	LEU	6.6
1	J	89	MET	6.4
1	K	251	GLY	6.3
1	K	214	LEU	6.2
1	J	222	GLY	6.1
1	K	283	LEU	6.0
1	J	223	LEU	5.9
1	K	295	ILE	5.7
1	H	287	THR	5.7
1	K	243	ILE	5.6
1	F	153	ILE	5.6
1	J	294	LEU	5.6
1	J	221	ALA	5.6
1	L	156	ILE	5.4
1	K	246	GLY	5.4
1	K	286	PHE	5.4
1	K	29	THR	5.4
1	K	270	ALA	5.4
1	K	90	ARG	5.4
1	F	228	GLY	5.3
1	K	66	HIS	5.3
1	G	85	PHE	5.3
1	H	224	MET	5.3
1	K	248	ILE	5.3
1	K	195	ASN	5.2
1	L	2	THR	5.2
1	K	201	VAL	5.2
1	J	287	THR	5.2
1	E	5	ARG	5.1
1	K	194	TYR	5.1
1	J	215	MET	5.1
1	J	3	LEU	5.0
1	F	89	MET	4.9
1	L	91	VAL	4.9
1	K	53	VAL	4.8
1	H	285	ILE	4.8
1	K	205	VAL	4.8
1	J	216	LEU	4.7

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Mol	Chain	Res	Type	RSRZ
1	F	190	ASN	4.7
1	K	22	ILE	4.7
1	F	248	ILE	4.6
1	L	142	THR	4.6
1	K	49	ALA	4.5
1	L	85	PHE	4.5
1	J	22	ILE	4.5
1	G	37	ASN	4.5
1	E	88	GLY	4.5
1	H	246	GLY	4.5
1	K	244	ALA	4.4
1	J	258	CYS	4.4
1	E	21	TYR	4.4
1	K	250	GLY	4.4
1	K	232	THR	4.4
1	K	4	SER	4.3
1	J	256	ILE	4.3
1	K	241	GLU	4.2
1	L	84	HIS	4.2
1	F	191	GLY	4.2
1	K	64	VAL	4.2
1	K	97	MET	4.2
1	I	143	ARG	4.1
1	J	91	VAL	4.1
1	J	72	ILE	4.1
1	J	285	ILE	4.1
1	K	269	SER	4.1
1	J	37	ASN	4.1
1	K	30	LEU	4.1
1	G	141	VAL	4.0
1	J	193	SER	4.0
1	K	193	SER	4.0
1	K	72	ILE	4.0
1	H	234	LEU	4.0
1	K	63	VAL	4.0
1	J	214	LEU	3.9
1	G	263	VAL	3.9
1	H	227	GLN	3.9
1	J	234	LEU	3.9
1	K	289	SER	3.8
1	J	293	THR	3.8
1	J	272	ILE	3.8

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Mol	Chain	Res	Type	RSRZ
1	G	147	GLU	3.8
1	K	182	ILE	3.8
1	K	260	LEU	3.8
1	H	275	GLY	3.8
1	J	282	LEU	3.8
1	H	218	THR	3.8
1	K	212	GLU	3.7
1	J	246	GLY	3.6
1	J	10	GLN	3.6
1	I	38	ALA	3.6
1	G	146	PRO	3.6
1	I	291	VAL	3.6
1	K	115	LEU	3.6
1	L	198	ALA	3.6
1	K	65	VAL	3.6
1	K	271	HIS	3.6
1	K	36	GLY	3.6
1	H	216	LEU	3.5
1	K	75	LEU	3.5
1	K	242	LEU	3.5
1	K	281	VAL	3.5
1	L	298	ARG	3.5
1	K	215	MET	3.5
1	B	2	THR	3.5
1	K	69	GLY	3.5
1	E	244	ALA	3.5
1	K	264	GLN	3.5
1	L	185	ILE	3.5
1	L	92	THR	3.4
1	J	248	ILE	3.4
1	H	293	THR	3.4
1	K	54	LEU	3.4
1	L	104	LEU	3.4
1	A	301	HIS	3.4
1	F	36	GLY	3.4
1	D	2	THR	3.4
1	J	260	LEU	3.3
1	K	200	LEU	3.3
1	G	5	ARG	3.3
1	L	39	MET	3.3
1	I	129	LYS	3.3
1	F	223	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	K	5	ARG	3.3
1	K	92	THR	3.3
1	L	86	ILE	3.3
1	K	198	ALA	3.3
1	J	134	ILE	3.2
1	K	196	ILE	3.2
1	L	159	VAL	3.2
1	J	270	ALA	3.2
1	F	35	GLY	3.2
1	H	36	GLY	3.2
1	L	297	ASN	3.2
1	K	37	ASN	3.2
1	L	229	GLN	3.2
1	J	224	MET	3.2
1	K	209	LEU	3.2
1	J	36	GLY	3.2
1	K	112	ILE	3.2
1	K	100	VAL	3.1
1	K	181	VAL	3.1
1	L	90	ARG	3.1
1	L	187	VAL	3.1
1	K	228	GLY	3.1
1	K	137	LYS	3.1
1	J	88	GLY	3.1
1	F	222	GLY	3.1
1	J	121	GLY	3.1
1	K	294	LEU	3.1
1	K	96	THR	3.1
1	K	225	ASP	3.1
1	J	58	VAL	3.1
1	I	256	ILE	3.1
1	E	272	ILE	3.0
1	F	144	GLN	3.0
1	L	144	GLN	3.0
1	J	23	ARG	3.0
1	J	247	THR	3.0
1	J	283	LEU	3.0
1	F	34	TYR	3.0
1	G	223	LEU	3.0
1	K	292	GLY	3.0
1	B	147	GLU	3.0
1	H	283	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	J	286	PHE	3.0
1	I	68	GLY	3.0
1	G	11	VAL	3.0
1	J	239	VAL	2.9
1	E	17	GLU	2.9
1	G	153	ILE	2.9
1	H	215	MET	2.9
1	F	96	THR	2.9
1	H	17	GLU	2.9
1	J	295	ILE	2.9
1	E	245	ASP	2.9
1	F	226	LYS	2.9
1	J	288	ASP	2.9
1	K	267	VAL	2.9
1	A	300	ARG	2.9
1	K	13	LYS	2.9
1	H	256	ILE	2.9
1	A	231	LEU	2.9
1	K	258	CYS	2.8
1	J	297	ASN	2.8
1	H	223	LEU	2.8
1	J	2	THR	2.8
1	K	290	GLY	2.8
1	K	249	TYR	2.8
1	L	8	ALA	2.8
1	K	32	ILE	2.8
1	K	116	ILE	2.8
1	L	3	LEU	2.8
1	G	148	MET	2.8
1	K	207	GLU	2.7
1	K	227	GLN	2.7
1	H	270	ALA	2.7
1	J	185	ILE	2.7
1	K	162	VAL	2.7
1	L	50	ARG	2.7
1	H	38	ALA	2.7
1	L	194	TYR	2.7
1	K	25	PHE	2.7
1	H	30	LEU	2.7
1	K	187	VAL	2.7
1	K	223	LEU	2.7
1	K	284	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	6	ASP	2.7
1	F	158	HIS	2.7
1	L	186	GLY	2.7
1	J	16	SER	2.7
1	E	13	LYS	2.7
1	K	8	ALA	2.7
1	G	217	LEU	2.6
1	K	131	ALA	2.6
1	J	271	HIS	2.6
1	E	296	SER	2.6
1	H	294	LEU	2.6
1	G	149	THR	2.6
1	J	25	PHE	2.6
1	I	89	MET	2.6
1	A	41	SER	2.6
1	J	187	VAL	2.6
1	K	83	SER	2.6
1	K	262	ALA	2.6
1	K	273	ILE	2.6
1	H	249	TYR	2.6
1	H	247	THR	2.6
1	L	89	MET	2.6
1	K	245	ASP	2.6
1	K	272	ILE	2.5
1	J	32	ILE	2.5
1	J	233	GLY	2.5
1	K	226	LYS	2.5
1	B	270	ALA	2.5
1	J	138	LYS	2.5
1	I	104	LEU	2.5
1	H	232	THR	2.5
1	K	202	ALA	2.5
1	H	260	LEU	2.5
1	K	114	ASN	2.5
1	F	239	VAL	2.5
1	J	158	HIS	2.5
1	J	232	THR	2.5
1	K	255	LYS	2.5
1	L	37	ASN	2.5
1	I	91	VAL	2.5
1	K	298	ARG	2.5
1	J	124	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	H	35	GLY	2.5
1	G	15	LEU	2.5
1	K	104	LEU	2.5
1	G	84	HIS	2.5
1	L	46	ALA	2.5
1	F	90	ARG	2.4
1	J	34	TYR	2.4
1	H	272	ILE	2.4
1	I	259	ALA	2.4
1	L	286	PHE	2.4
1	J	35	GLY	2.4
1	G	154	ILE	2.4
1	J	289	SER	2.4
1	H	6	ASP	2.4
1	L	109	ASN	2.4
1	K	185	ILE	2.3
1	L	295	ILE	2.3
1	J	200	LEU	2.3
1	J	14	VAL	2.3
1	E	7	ASP	2.3
1	J	194	TYR	2.3
1	A	8	ALA	2.3
1	L	55	MET	2.3
1	J	60	ILE	2.3
1	A	290	GLY	2.3
1	F	68	GLY	2.3
1	G	299	LYS	2.3
1	C	222	GLY	2.3
1	J	205	VAL	2.3
1	H	217	LEU	2.3
1	J	253	LEU	2.3
1	B	259	ALA	2.3
1	I	42	GLU	2.3
1	K	268	THR	2.3
1	H	282	LEU	2.2
1	J	21	TYR	2.2
1	H	233	GLY	2.2
1	J	54	LEU	2.2
1	E	287	THR	2.2
1	L	44	LEU	2.2
1	F	193	SER	2.2
1	K	160	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	J	292	GLY	2.2
1	L	299	LYS	2.2
1	B	248	ILE	2.2
1	G	256	ILE	2.2
1	J	90	ARG	2.2
1	A	11	VAL	2.2
1	E	100	VAL	2.2
1	G	83	SER	2.1
1	K	105	GLY	2.1
1	I	98	ASP	2.1
1	A	295	ILE	2.1
1	B	239	VAL	2.1
1	F	138	LYS	2.1
1	K	76	LEU	2.1
1	I	165	VAL	2.1
1	G	124	ILE	2.1
1	J	9	ALA	2.1
1	H	115	LEU	2.1
1	H	5	ARG	2.1
1	G	3	LEU	2.1
1	J	252	MET	2.1
1	H	269	SER	2.1
1	E	271	HIS	2.1
1	G	82	GLU	2.1
1	B	234	LEU	2.0
1	J	218	THR	2.0
1	K	183	ALA	2.0
1	B	148	MET	2.0
1	J	11	VAL	2.0
1	E	288	ASP	2.0
1	E	142	THR	2.0
1	G	150	LYS	2.0
1	J	268	THR	2.0
1	K	7	ASP	2.0
1	F	152	GLU	2.0
1	F	237	GLU	2.0
1	G	34	TYR	2.0
1	H	21	TYR	2.0
1	K	58	VAL	2.0
1	K	118	ARG	2.0
1	J	137	LYS	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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.

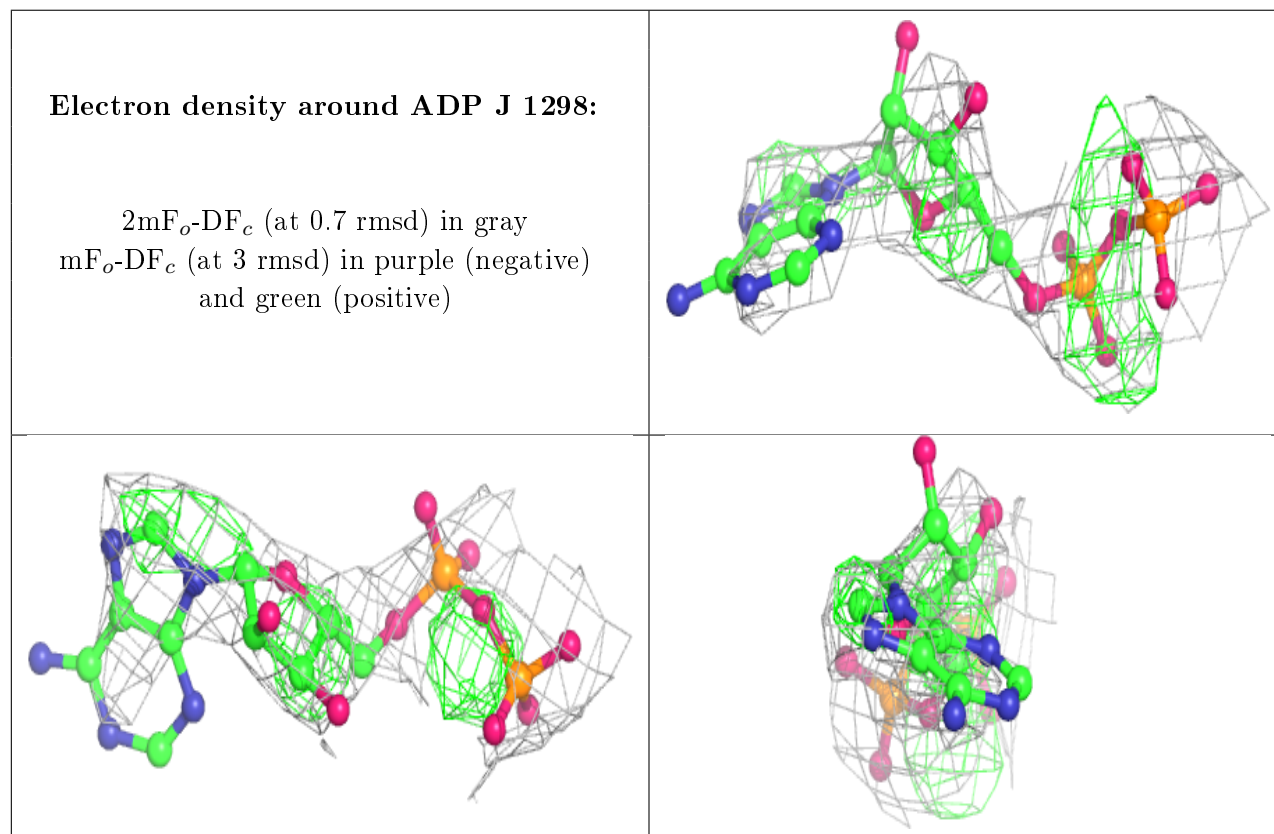
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NLG	F	1300	13/13	0.38	1.05	119,119,120,120	13
2	NLG	K	1298	13/13	0.57	0.97	100,101,102,103	13
3	ADP	J	1298	27/27	0.64	0.37	123,124,125,125	27
2	NLG	H	1299	13/13	0.64	0.51	115,116,118,118	13
5	CL	L	1303	1/1	0.67	0.26	100,100,100,100	0
3	ADP	H	1297	27/27	0.67	0.42	120,121,122,122	27
2	NLG	L	1302	13/13	0.71	0.35	108,110,112,112	0
5	CL	G	1302	1/1	0.71	0.22	92,92,92,92	0
2	NLG	G	1301	13/13	0.75	0.30	91,95,99,99	13
4	MG	H	1298	1/1	0.78	0.13	94,94,94,94	0
5	CL	H	1300	1/1	0.80	0.10	97,97,97,97	0
4	MG	C	1301	1/1	0.82	0.28	110,110,110,110	0
4	MG	I	1299	1/1	0.85	0.17	74,74,74,74	0
4	MG	E	1300	1/1	0.86	0.29	69,69,69,69	0
4	MG	L	1301	1/1	0.86	0.27	68,68,68,68	0
3	ADP	C	1300	27/27	0.88	0.28	70,90,117,118	0
3	ADP	G	1299	27/27	0.88	0.25	83,93,120,120	0
2	NLG	I	1300	13/13	0.88	0.37	93,95,96,96	0
2	NLG	E	1301	13/13	0.90	0.34	79,83,86,86	0
5	CL	D	1303	1/1	0.91	0.24	86,86,86,86	0
3	ADP	F	1299	27/27	0.91	0.18	103,109,124,125	0
2	NLG	A	1302	13/13	0.91	0.26	75,78,82,82	0
2	NLG	D	1302	13/13	0.92	0.34	56,58,61,64	0
5	CL	B	1303	1/1	0.93	0.18	82,82,82,82	0
3	ADP	L	1300	27/27	0.93	0.19	68,76,90,92	0
2	NLG	B	1302	13/13	0.94	0.24	57,64,66,68	0
3	ADP	I	1298	27/27	0.94	0.20	48,53,82,84	0

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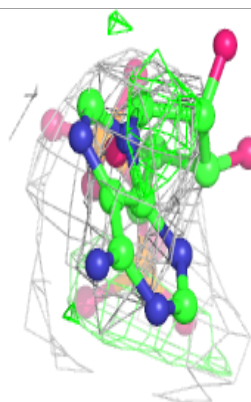
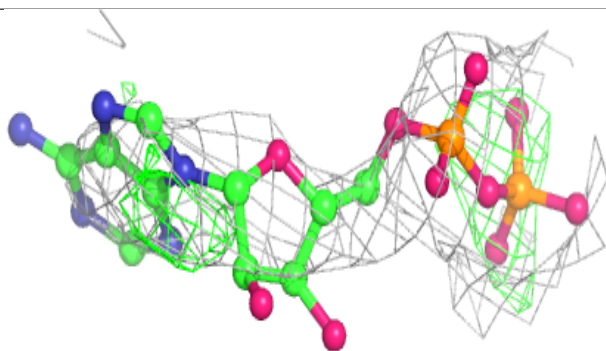
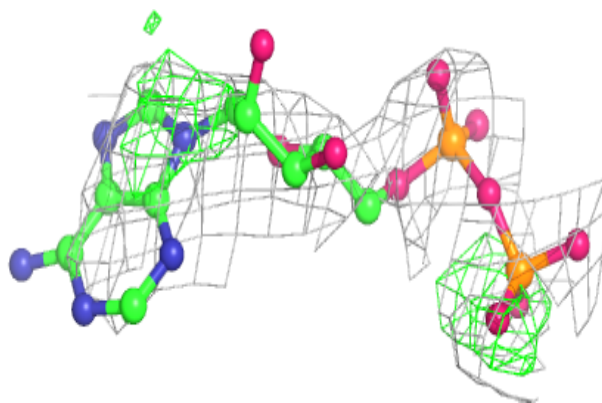
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	ADP	E	1299	27/27	0.94	0.20	55,64,77,77	0
4	MG	D	1301	1/1	0.95	0.21	56,56,56,56	0
3	ADP	B	1300	27/27	0.96	0.18	62,68,71,72	0
3	ADP	D	1300	27/27	0.97	0.18	43,48,58,59	0
5	CL	C	1302	1/1	0.97	0.12	84,84,84,84	0
4	MG	B	1301	1/1	0.98	0.32	50,50,50,50	0
4	MG	G	1300	1/1	0.98	0.20	85,85,85,85	0

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

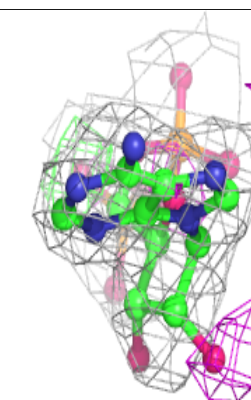
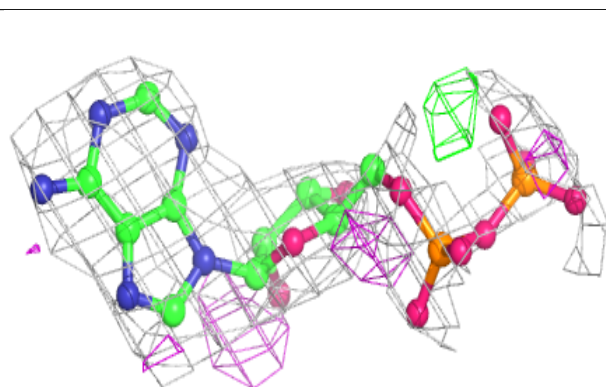
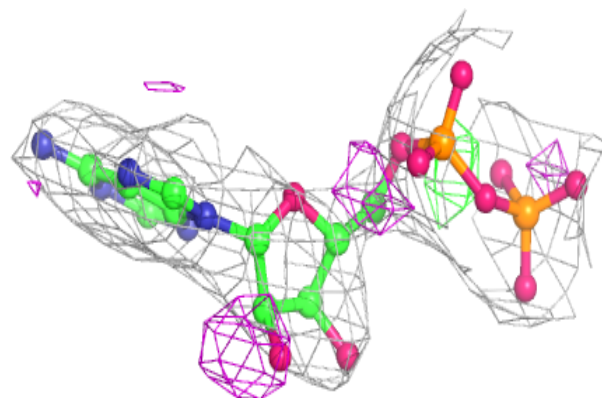


**Electron density around ADP H 1297:**

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

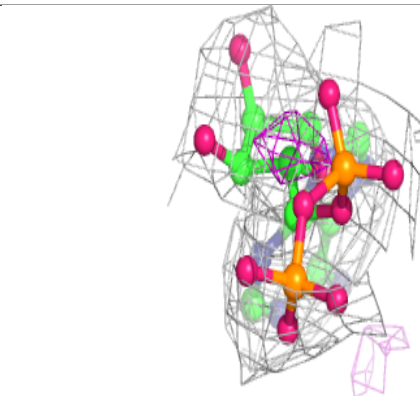
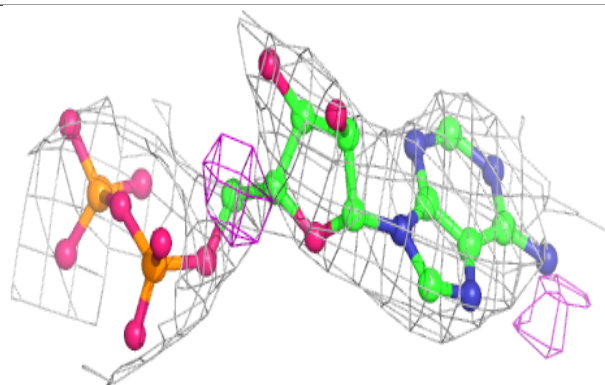
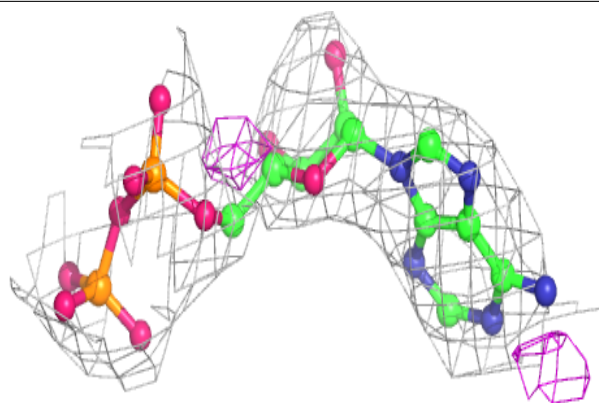
**Electron density around ADP C 1300:**

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

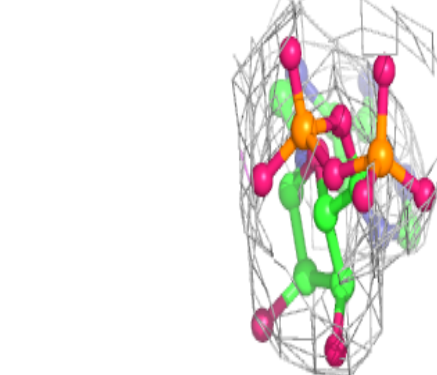
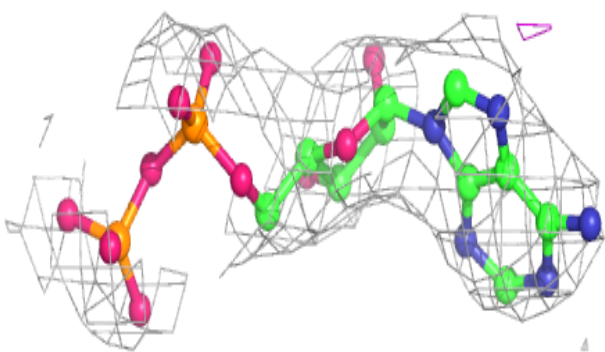
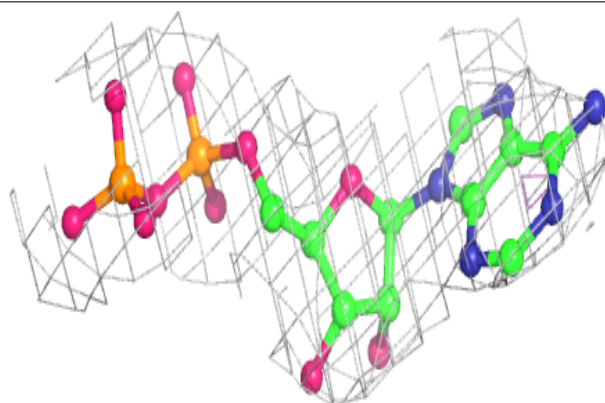


**Electron density around ADP G 1299:**

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

**Electron density around ADP F 1299:**

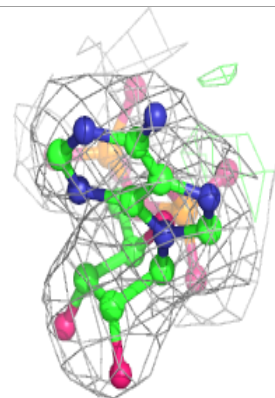
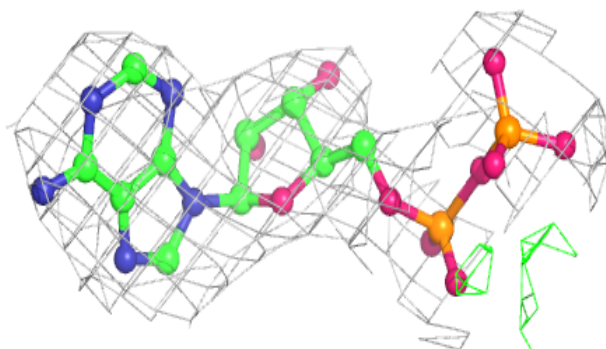
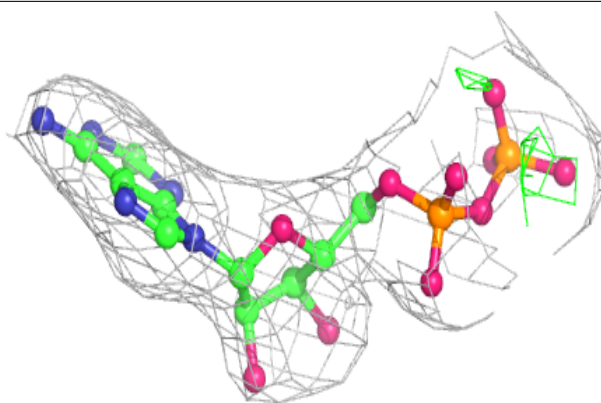
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



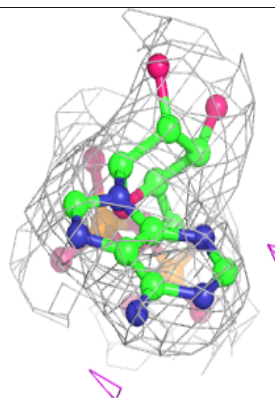
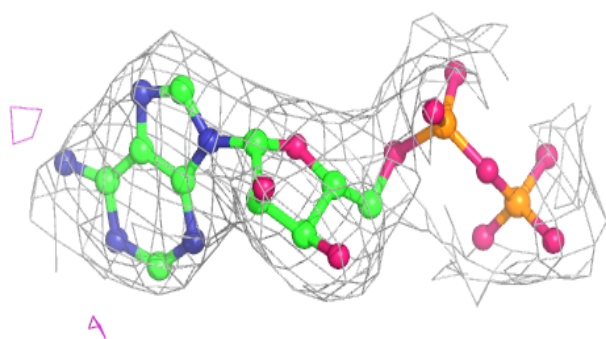
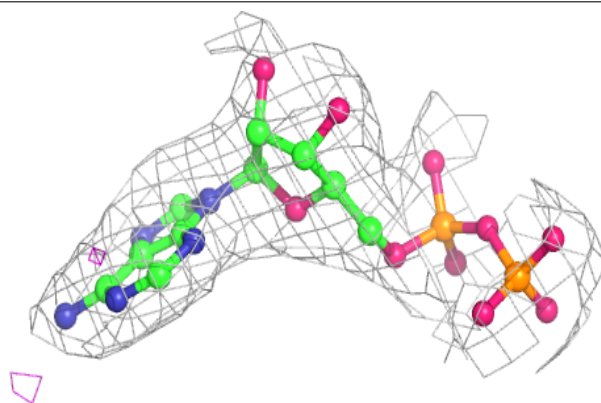


**Electron density around ADP L 1300:**

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

**Electron density around ADP I 1298:**

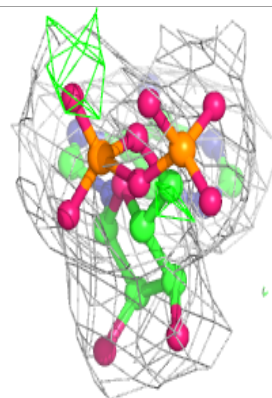
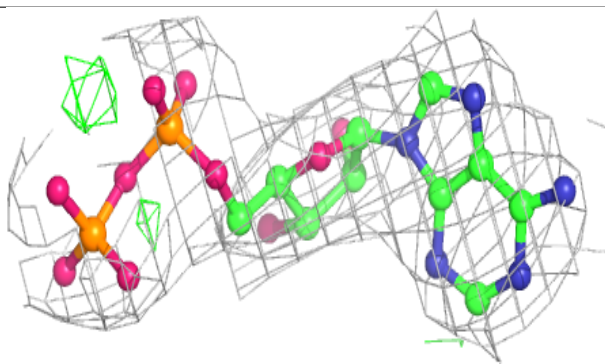
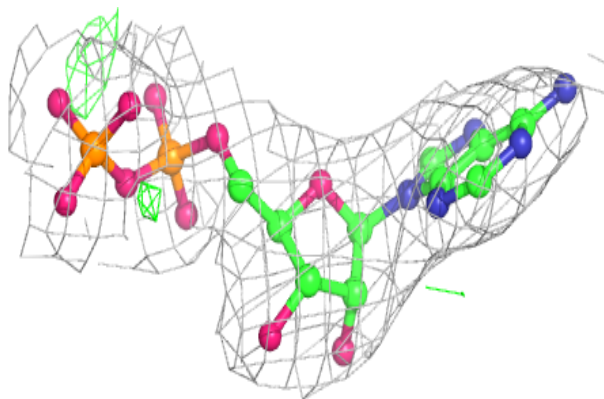
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



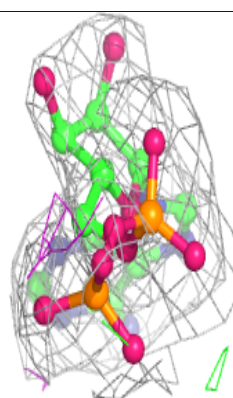
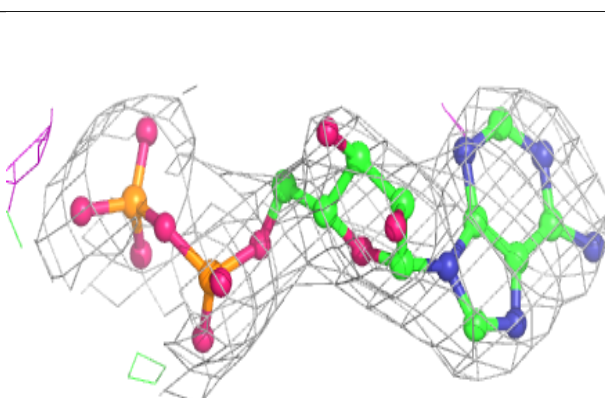
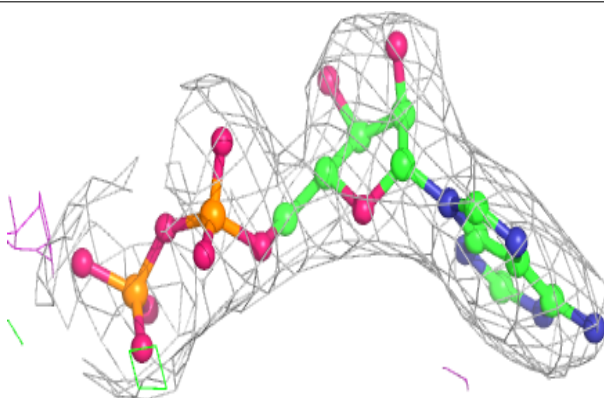


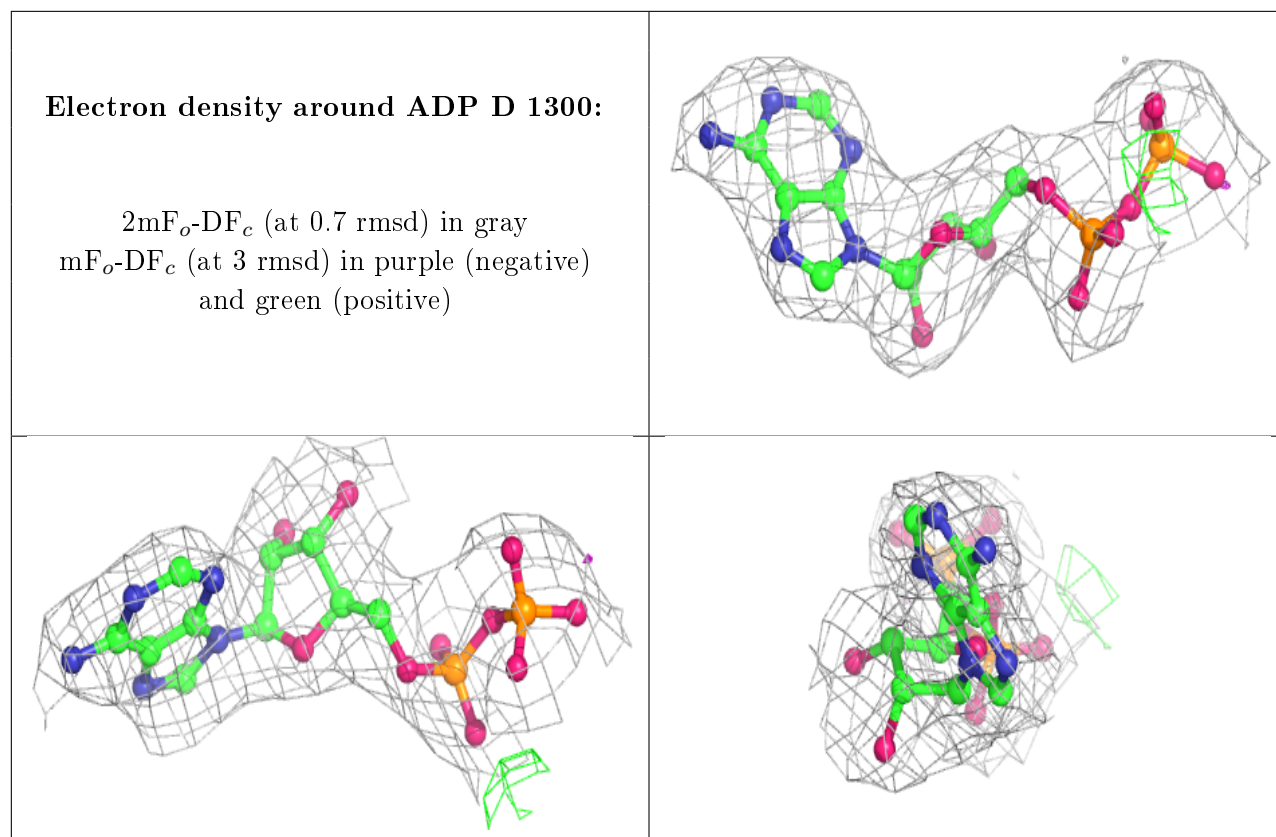
**Electron density around ADP E 1299:**

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

**Electron density around ADP B 1300:**

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





## 6.5 Other polymers [i](#)

There are no such residues in this entry.