



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 07:48 AM UTC

PDB ID : 2BUF / pdb\_00002buf  
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.

The types of validation reports are described at

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

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

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

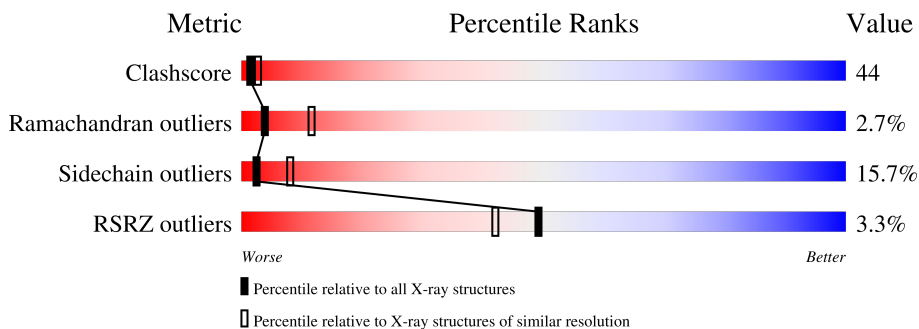
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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 style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 39%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 43%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 14%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">2% 39% 43% 14% . .</p>
1	B	300	<div style="display: flex; align-items: center;"> <div style="width: 40%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 48%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 10%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">40% 48% 10% ..</p>
1	C	300	<div style="display: flex; align-items: center;"> <div style="width: 52%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 36%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 11%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">52% 36% 11% .</p>
1	D	300	<div style="display: flex; align-items: center;"> <div style="width: 56%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 32%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 9%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">56% 32% 9% ..</p>
1	E	300	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 39%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 43%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 11%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">2% 40% 43% 11% . .</p>
1	F	300	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 40%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 43%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 12%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">2% 40% 43% 12% . .</p>
1	G	300	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 45%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 39%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 13%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">2% 45% 39% 13% ..</p>

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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	G	1301	-	X	-	-
2	NLG	H	1299	-	X	X	-
2	NLG	I	1300	-	X	-	-
2	NLG	K	1298	-	X	-	-
2	NLG	L	1302	-	X	-	-
3	ADP	J	1298	-	-	X	-

## 2 Entry composition

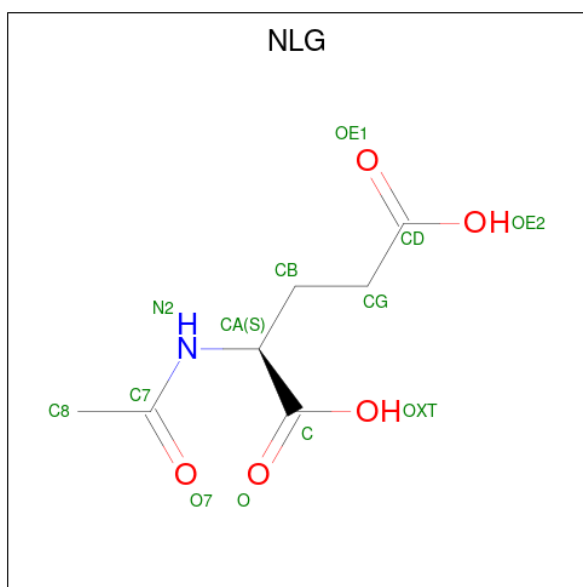
There are 5 unique types of molecules in this entry. The entry contains 25923 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

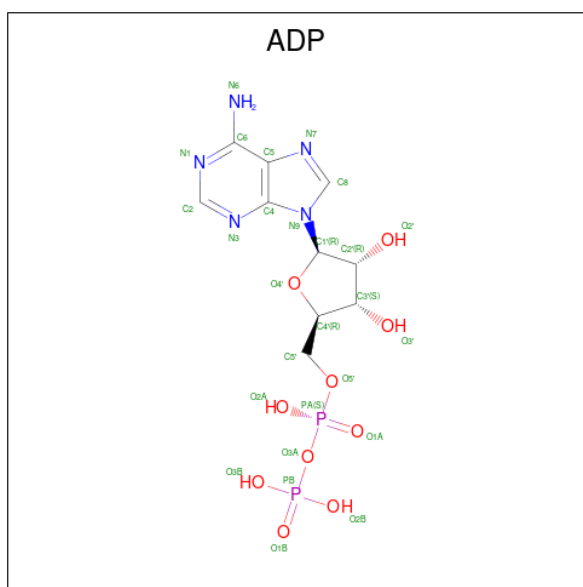
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	292	Total 2159	C 1359	N 382	O 408	S 10	0	0	0
1	B	297	Total 2177	C 1371	N 379	O 416	S 11	0	0	1
1	C	299	Total 2201	C 1386	N 385	O 419	S 11	0	0	1
1	D	295	Total 2170	C 1367	N 381	O 412	S 10	0	0	1
1	E	288	Total 2106	C 1327	N 368	O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

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



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

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
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 (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
4	B	1	Total	Mg	0	0
			1	1		
4	C	1	Total	Mg	0	0
			1	1		

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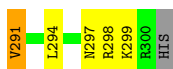
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	1	Total Mg 1 1	0	0
4	E	1	Total Mg 1 1	0	0
4	G	1	Total Mg 1 1	0	0
4	H	1	Total Mg 1 1	0	0
4	I	1	Total Mg 1 1	0	0
4	L	1	Total Mg 1 1	0	0

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

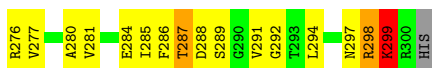
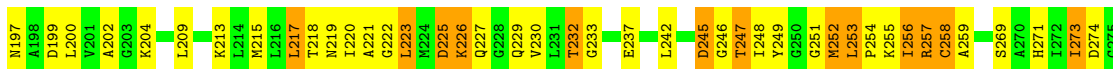
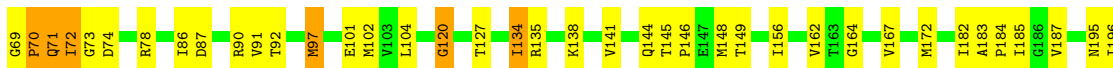
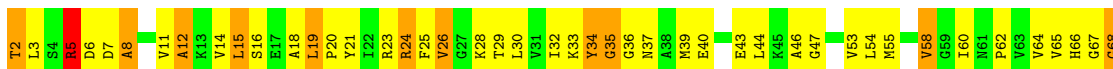
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total Cl 1 1	0	0
5	C	1	Total Cl 1 1	0	0
5	D	1	Total Cl 1 1	0	0
5	G	1	Total Cl 1 1	0	0
5	H	1	Total Cl 1 1	0	0
5	L	1	Total Cl 1 1	0	0





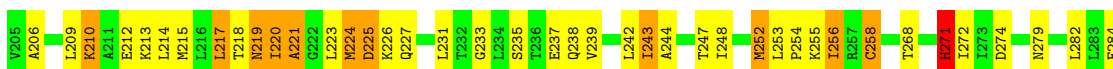
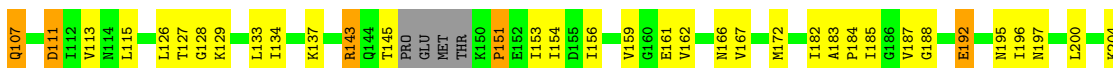
- Molecule 1: ACETYLGLUTAMATE KINASE

Chain C: 52% 36% 11%



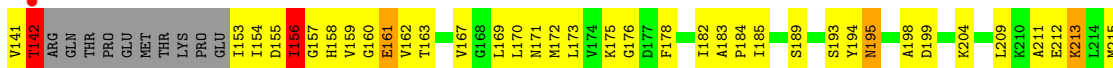
- Molecule 1: ACETYLGLUTAMATE KINASE

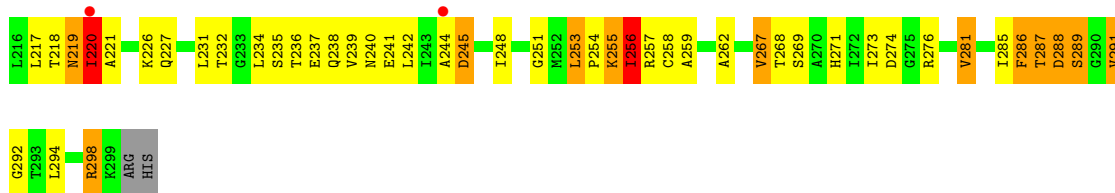
Chain D: 56% 32% 9%



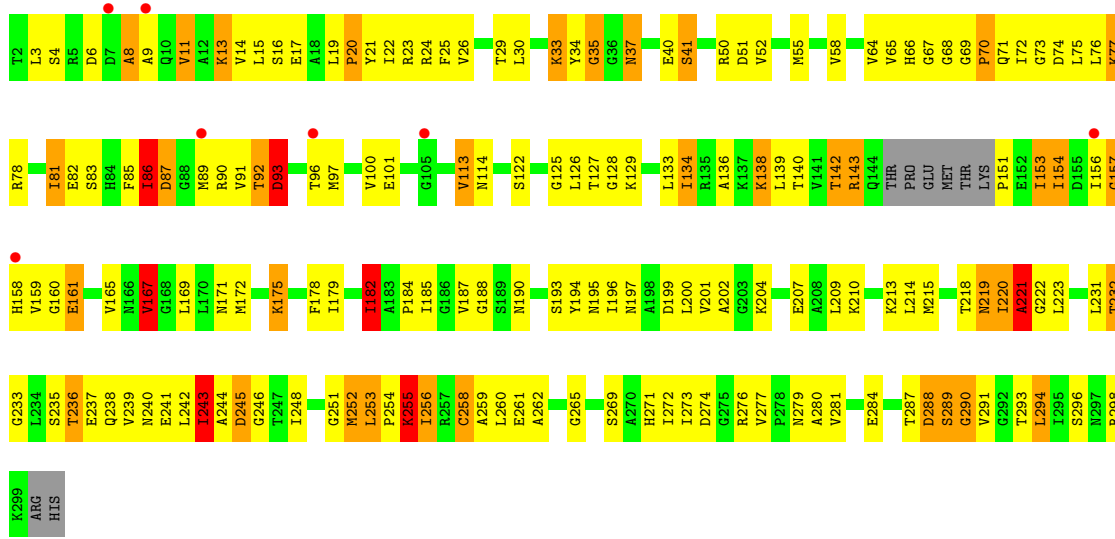
- Molecule 1: ACETYLGLUTAMATE KINASE

Chain E: 2% 40% 43% 11%

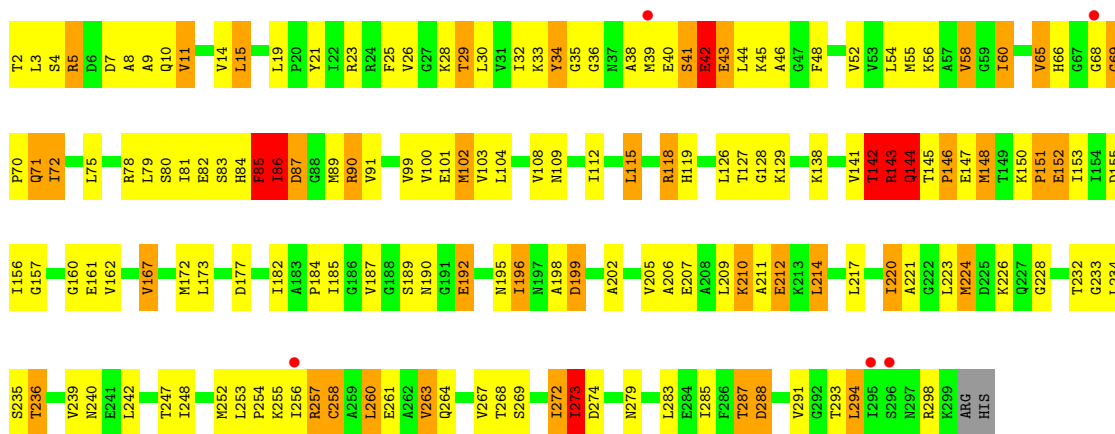




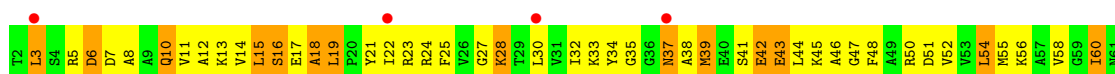
● Molecule 1: ACETYLGLUTAMATE KINASE

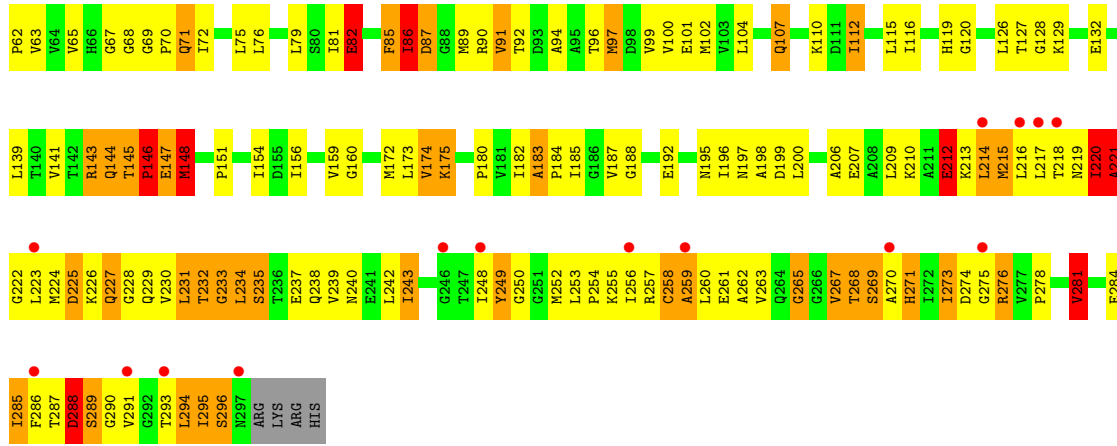


● Molecule 1: ACETYLGLUTAMATE KINASE

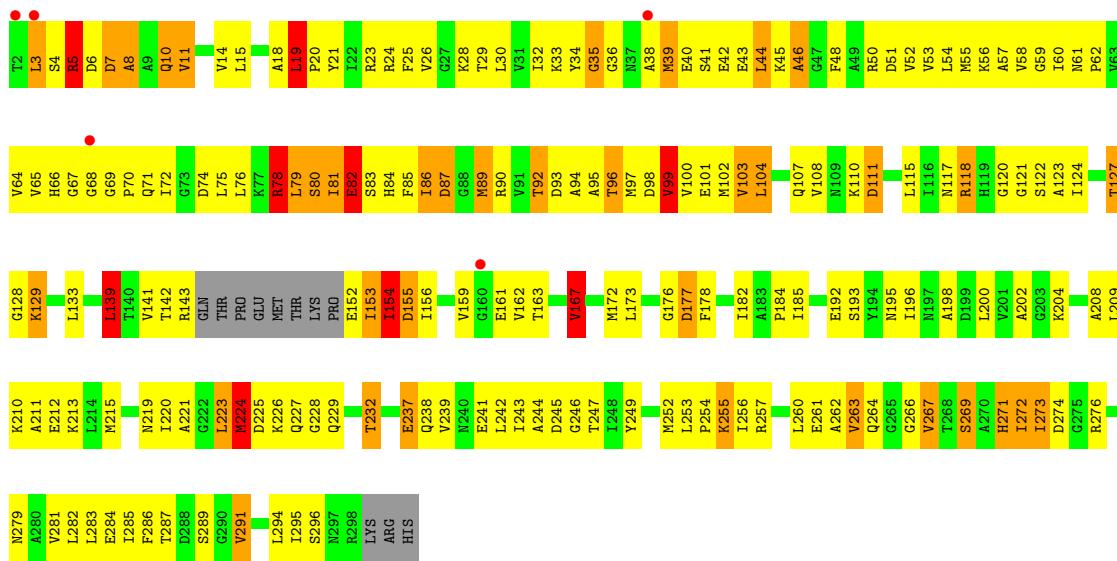


● Molecule 1: ACETYLGLUTAMATE KINASE

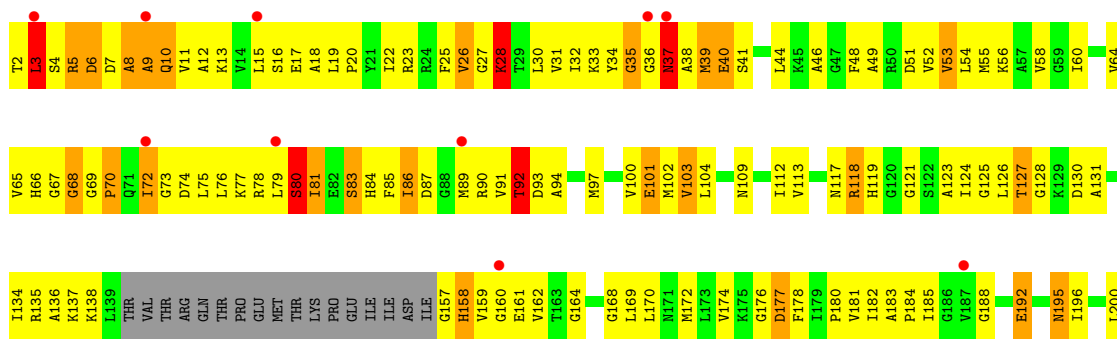




• Molecule 1: ACETYLGLUTAMATE KINASE



• Molecule 1: ACETYLGLUTAMATE KINASE





## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	71.86Å 98.78Å 162.90Å 91.49° 92.03° 107.56°	Depositor
Resolution (Å)	18.00 – 2.95 18.00 – 2.95	Depositor EDS
% Data completeness (in resolution range)	96.7 (18.00-2.95) 96.2 (18.00-2.95)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.73 (at 2.82Å)	Xtrriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.249 , 0.267 0.245 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	78.7	Xtrriage
Anisotropy	0.093	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 62.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.009 for -h,-k,l	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	25923	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	88.0	wwPDB-VP

Xtrriage'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 i

### 5.1 Standard geometry i

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

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	0.73	1/2179 (0.0%)	1.33	34/2940 (1.2%)
1	B	0.74	1/2197 (0.0%)	1.38	28/2969 (0.9%)
1	C	0.76	2/2223 (0.1%)	1.25	19/3005 (0.6%)
1	D	0.77	3/2190 (0.1%)	1.31	21/2958 (0.7%)
1	E	0.75	4/2125 (0.2%)	1.40	39/2872 (1.4%)
1	F	0.62	1/2151 (0.0%)	1.29	32/2907 (1.1%)
1	G	0.66	2/2208 (0.1%)	1.34	31/2987 (1.0%)
1	H	0.74	4/2195 (0.2%)	1.47	46/2969 (1.5%)
1	I	0.71	0/2129	1.42	42/2878 (1.5%)
1	J	0.71	3/2033 (0.1%)	1.36	30/2747 (1.1%)
1	K	0.83	6/1934 (0.3%)	1.38	38/2620 (1.5%)
1	L	0.68	0/2183	1.31	33/2948 (1.1%)
All	All	0.73	27/25747 (0.1%)	1.35	393/34800 (1.1%)

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 (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	138	LYS	N-CA	16.81	1.67	1.45
1	K	137	LYS	CA-C	10.53	1.67	1.52
1	E	4	SER	C-O	-8.96	1.12	1.24
1	D	252	MET	SD-CE	-7.62	1.60	1.79
1	H	91	VAL	CA-CB	-7.17	1.45	1.54
1	K	138	LYS	CA-CB	6.92	1.63	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	298	ARG	C-N	-6.60	1.24	1.33
1	C	97	MET	SD-CE	-6.55	1.63	1.79
1	E	5	ARG	N-CA	-6.55	1.37	1.46
1	K	137	LYS	N-CA	6.50	1.55	1.46
1	K	138	LYS	CA-C	6.32	1.61	1.53
1	A	97	MET	SD-CE	-5.90	1.64	1.79
1	D	298	ARG	CA-C	5.72	1.59	1.52
1	G	143	ARG	CA-C	-5.67	1.45	1.52
1	H	296	SER	C-N	-5.49	1.25	1.33
1	F	298	ARG	C-N	-5.49	1.25	1.33
1	B	299	LYS	C-N	-5.40	1.25	1.33
1	J	297	ASN	C-N	-5.34	1.25	1.33
1	H	87	ASP	CA-C	-5.33	1.47	1.53
1	D	299	LYS	C-N	-5.32	1.25	1.33
1	E	298	ARG	C-N	-5.30	1.25	1.33
1	K	297	ASN	C-N	-5.30	1.25	1.33
1	C	299	LYS	C-N	-5.29	1.25	1.33
1	J	35	GLY	CA-C	-5.29	1.45	1.52
1	E	5	ARG	CA-CB	-5.24	1.44	1.53
1	J	220	ILE	CG1-CD1	-5.18	1.31	1.51
1	H	91	VAL	N-CA	-5.08	1.40	1.46

All (393) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	149	THR	N-CA-C	18.14	138.78	109.95
1	E	3	LEU	N-CA-C	-14.65	90.04	113.19
1	D	298	ARG	N-CA-C	-14.37	86.20	109.76
1	I	96	THR	N-CA-C	-13.52	97.25	113.88
1	D	8	ALA	N-CA-C	-12.98	95.89	112.90
1	A	42	GLU	N-CA-C	12.88	127.85	111.24
1	J	8	ALA	N-CA-C	-12.02	98.32	113.23
1	C	5	ARG	N-CA-C	-11.34	98.93	111.07
1	H	276	ARG	N-CA-C	-11.26	99.08	113.72
1	G	87	ASP	N-CA-C	10.95	127.14	112.25
1	K	233	GLY	N-CA-C	10.95	130.71	115.27
1	E	81	ILE	N-CA-C	10.85	120.62	110.42
1	J	4	SER	N-CA-C	-10.25	97.31	110.53
1	J	28	LYS	N-CA-C	10.10	124.19	110.55
1	K	4	SER	N-CA-C	9.57	131.19	110.80
1	H	148	MET	N-CA-C	9.51	131.06	110.80
1	K	234	LEU	N-CA-C	9.46	122.53	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	37	ASN	N-CA-C	-9.43	101.46	113.72
1	B	225	ASP	N-CA-C	-9.37	97.00	110.59
1	C	288	ASP	N-CA-C	-9.35	101.88	113.20
1	F	182	ILE	N-CA-C	9.33	121.33	107.80
1	E	298	ARG	N-CA-C	9.28	136.97	111.00
1	G	38	ALA	N-CA-C	-9.21	102.04	113.28
1	D	226	LYS	N-CA-C	-9.12	101.92	113.23
1	F	245	ASP	N-CA-C	-9.12	100.48	112.34
1	A	247	THR	N-CA-C	-9.11	101.88	113.72
1	E	288	ASP	N-CA-C	-9.09	99.25	110.61
1	K	25	PHE	N-CA-C	8.92	124.16	113.28
1	L	8	ALA	N-CA-C	-8.82	92.00	110.80
1	I	44	LEU	N-CA-C	-8.80	102.55	113.38
1	J	225	ASP	N-CA-C	-8.76	98.44	110.35
1	B	182	ILE	N-CA-C	8.67	120.41	107.75
1	F	157	GLY	N-CA-C	-8.64	100.74	112.57
1	L	246	GLY	N-CA-C	-8.64	103.03	115.64
1	E	94	ALA	N-CA-C	8.53	121.43	111.02
1	A	232	THR	N-CA-C	8.42	123.83	111.96
1	L	298	ARG	N-CA-C	-8.42	95.82	109.96
1	B	3	LEU	N-CA-C	8.30	123.29	110.42
1	B	40	GLU	N-CA-C	8.30	128.47	110.80
1	I	267	VAL	N-CA-C	8.30	120.43	108.48
1	H	183	ALA	CA-C-N	8.29	130.20	119.84
1	H	183	ALA	C-N-CA	8.29	130.20	119.84
1	G	196	ILE	N-CA-C	8.28	118.65	108.06
1	A	88	GLY	N-CA-C	-8.27	103.61	115.27
1	H	19	LEU	N-CA-C	8.25	128.04	109.81
1	L	5	ARG	N-CA-C	-8.22	103.25	113.28
1	I	80	SER	CA-C-N	8.21	134.18	122.77
1	I	80	SER	C-N-CA	8.21	134.18	122.77
1	H	198	ALA	N-CA-C	8.21	121.15	111.71
1	H	182	ILE	N-CA-C	8.10	120.36	107.73
1	E	182	ILE	N-CA-C	8.03	119.47	107.51
1	H	285	ILE	N-CA-C	7.99	119.78	112.43
1	A	91	VAL	N-CA-C	-7.98	98.14	109.63
1	F	86	ILE	N-CA-C	7.98	125.94	109.34
1	I	99	VAL	N-CA-C	-7.97	104.04	111.45
1	J	103	VAL	N-CA-C	7.93	117.88	110.42
1	A	273	ILE	N-CA-C	7.87	121.27	108.99
1	K	112	ILE	N-CA-C	-7.80	102.93	110.42
1	C	34	TYR	N-CA-C	-7.79	98.69	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	243	ILE	N-CA-C	-7.70	102.95	110.72
1	G	288	ASP	N-CA-C	-7.68	98.89	109.71
1	H	19	LEU	CA-C-N	-7.67	110.25	119.84
1	H	19	LEU	C-N-CA	-7.67	110.25	119.84
1	E	3	LEU	CA-C-N	7.67	136.18	121.54
1	E	3	LEU	C-N-CA	7.67	136.18	121.54
1	D	69	GLY	CA-C-N	7.64	127.19	119.24
1	D	69	GLY	C-N-CA	7.64	127.19	119.24
1	J	168	GLY	N-CA-C	-7.64	103.63	112.50
1	I	154	ILE	N-CA-C	7.64	118.92	108.84
1	H	291	VAL	N-CA-C	-7.62	99.74	109.58
1	H	288	ASP	N-CA-C	-7.62	94.58	110.80
1	K	91	VAL	N-CA-C	-7.60	99.11	109.37
1	I	182	ILE	N-CA-C	7.54	119.44	108.58
1	I	43	GLU	N-CA-C	7.53	122.23	112.89
1	I	8	ALA	N-CA-C	7.53	120.55	111.82
1	I	291	VAL	N-CA-C	-7.51	97.02	107.99
1	H	71	GLN	N-CA-C	-7.50	104.10	113.18
1	E	15	LEU	N-CA-C	-7.50	103.19	111.36
1	H	15	LEU	N-CA-C	-7.44	102.85	112.23
1	K	137	LYS	CA-C-O	-7.44	112.86	121.49
1	A	289	SER	N-CA-C	-7.43	100.27	111.34
1	J	9	ALA	N-CA-C	-7.39	103.22	112.90
1	C	225	ASP	N-CA-C	-7.38	99.59	110.52
1	C	70	PRO	N-CA-C	-7.38	105.24	114.68
1	B	233	GLY	N-CA-C	7.37	125.59	114.61
1	A	182	ILE	N-CA-C	7.35	118.72	107.99
1	G	145	THR	N-CA-C	-7.34	93.59	109.81
1	J	56	LYS	N-CA-C	7.33	120.70	111.69
1	F	290	GLY	N-CA-C	-7.32	95.84	113.18
1	A	142	THR	N-CA-C	-7.30	99.10	110.42
1	L	153	ILE	N-CA-C	7.30	119.00	109.58
1	J	222	GLY	N-CA-C	-7.29	100.65	110.56
1	I	127	THR	N-CA-C	-7.26	98.27	109.52
1	H	226	LYS	N-CA-C	7.25	122.25	111.81
1	B	94	ALA	N-CA-C	7.25	119.81	111.11
1	F	41	SER	N-CA-C	-7.21	100.82	110.55
1	F	276	ARG	N-CA-C	-7.17	104.15	113.12
1	H	212	GLU	N-CA-C	-7.17	103.99	112.89
1	L	268	THR	N-CA-C	7.16	120.12	111.82
1	L	108	VAL	N-CA-C	7.16	117.92	110.62
1	G	41	SER	N-CA-C	-7.14	100.50	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	39	MET	N-CA-C	-7.13	104.59	112.72
1	L	136	ALA	N-CA-C	7.11	119.99	108.76
1	J	81	ILE	N-CA-C	7.09	117.62	108.12
1	H	220	ILE	N-CA-C	-7.06	94.66	109.34
1	J	85	PHE	N-CA-C	7.06	119.85	109.69
1	B	285	ILE	N-CA-C	7.04	119.04	111.58
1	C	246	GLY	N-CA-C	7.04	123.06	114.69
1	D	36	GLY	N-CA-C	-7.03	106.27	115.47
1	L	264	GLN	N-CA-C	-7.02	104.19	112.89
1	H	86	ILE	N-CA-C	7.01	123.91	109.34
1	K	69	GLY	CA-C-N	6.99	128.58	119.84
1	K	69	GLY	C-N-CA	6.99	128.58	119.84
1	L	182	ILE	N-CA-C	6.97	118.16	107.99
1	G	143	ARG	N-CA-C	6.96	125.62	110.80
1	C	72	ILE	N-CA-C	-6.96	104.98	111.45
1	A	86	ILE	CB-CA-C	-6.94	99.91	111.29
1	C	182	ILE	N-CA-C	6.94	118.28	108.36
1	L	260	LEU	N-CA-C	-6.88	102.88	112.45
1	H	28	LYS	N-CA-C	6.81	120.47	110.59
1	G	5	ARG	N-CA-C	-6.81	103.92	111.82
1	L	37	ASN	N-CA-C	-6.79	103.11	111.33
1	G	42	GLU	N-CA-C	6.79	121.95	111.56
1	L	36	GLY	N-CA-C	-6.78	105.54	115.30
1	H	174	VAL	N-CA-C	6.77	118.33	110.62
1	K	64	VAL	N-CA-C	6.75	119.14	108.87
1	I	35	GLY	N-CA-C	-6.74	105.55	111.95
1	L	91	VAL	N-CA-C	-6.73	100.28	109.37
1	A	292	GLY	N-CA-C	-6.72	101.33	110.20
1	E	3	LEU	CA-C-O	6.72	126.00	119.08
1	I	224	MET	N-CA-C	6.71	120.07	109.81
1	G	34	TYR	CB-CA-C	-6.67	100.55	111.68
1	E	271	HIS	N-CA-C	6.66	119.27	108.41
1	D	296	SER	N-CA-C	-6.66	97.75	109.06
1	F	70	PRO	N-CA-C	-6.65	104.86	113.57
1	C	35	GLY	N-CA-C	-6.62	97.48	113.18
1	K	137	LYS	O-C-N	6.62	131.88	122.74
1	C	8	ALA	N-CA-C	-6.61	105.35	113.41
1	E	38	ALA	N-CA-C	-6.60	105.19	113.18
1	D	38	ALA	N-CA-C	6.59	124.85	110.80
1	G	264	GLN	N-CA-C	-6.59	105.10	113.01
1	F	34	TYR	N-CA-C	6.58	121.68	112.93
1	H	112	ILE	N-CA-C	-6.58	103.91	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	182	ILE	N-CA-C	6.56	117.36	108.17
1	H	295	ILE	N-CA-C	6.55	119.53	108.86
1	H	6	ASP	N-CA-C	6.55	118.30	111.03
1	G	273	ILE	N-CA-C	6.54	119.76	108.90
1	D	43	GLU	N-CA-C	-6.53	104.57	112.54
1	B	148	MET	N-CA-C	-6.53	94.23	107.41
1	E	142	THR	N-CA-C	6.52	129.26	111.00
1	F	92	THR	N-CA-C	6.51	118.89	108.41
1	J	94	ALA	N-CA-C	6.49	118.90	111.11
1	F	136	ALA	N-CA-C	6.48	118.00	108.86
1	H	145	THR	CA-C-N	6.47	127.93	119.84
1	H	145	THR	C-N-CA	6.47	127.93	119.84
1	G	182	ILE	N-CA-C	6.46	117.60	108.36
1	D	4	SER	N-CA-C	-6.42	99.82	109.96
1	D	271	HIS	N-CA-C	6.41	119.95	109.24
1	F	64	VAL	N-CA-C	6.41	117.53	108.36
1	C	257	ARG	N-CA-C	-6.38	104.33	111.28
1	H	284	GLU	N-CA-C	6.37	120.52	112.87
1	B	67	GLY	N-CA-C	-6.37	105.15	112.79
1	B	297	ASN	N-CA-C	-6.33	105.02	114.64
1	G	65	VAL	N-CA-C	-6.32	99.11	108.85
1	I	64	VAL	N-CA-C	6.31	116.71	107.37
1	I	269	SER	N-CA-C	6.31	118.11	108.52
1	H	273	ILE	N-CA-C	6.30	119.36	108.90
1	J	243	ILE	N-CA-C	-6.30	103.75	110.36
1	F	252	MET	N-CA-C	-6.29	105.25	113.12
1	H	225	ASP	N-CA-C	-6.29	100.38	109.31
1	L	187	VAL	N-CA-C	6.28	116.91	107.75
1	A	114	ASN	N-CA-C	-6.27	104.36	111.07
1	J	277	VAL	N-CA-C	6.26	114.01	108.63
1	I	83	SER	N-CA-C	6.26	120.26	107.69
1	J	10	GLN	N-CA-C	-6.24	104.10	111.03
1	F	69	GLY	CA-C-N	-6.23	112.58	119.19
1	F	69	GLY	C-N-CA	-6.23	112.58	119.19
1	I	46	ALA	N-CA-C	-6.23	104.57	111.36
1	J	53	VAL	N-CA-C	-6.21	104.23	111.00
1	F	8	ALA	N-CA-C	-6.21	103.66	111.11
1	L	82	GLU	N-CA-C	6.21	124.02	110.80
1	G	148	MET	CA-C-N	6.20	128.87	120.38
1	G	148	MET	C-N-CA	6.20	128.87	120.38
1	H	86	ILE	CA-C-N	-6.19	114.50	122.79
1	H	86	ILE	C-N-CA	-6.19	114.50	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	80	SER	N-CA-C	6.19	123.98	110.80
1	G	86	ILE	CA-C-N	-6.16	112.72	122.95
1	G	86	ILE	C-N-CA	-6.16	112.72	122.95
1	F	25	PHE	N-CA-C	6.15	120.40	113.02
1	I	18	ALA	N-CA-C	-6.12	104.88	112.90
1	A	32	ILE	N-CA-C	6.12	116.19	106.88
1	H	89	MET	N-CA-C	6.11	119.67	109.95
1	K	138	LYS	CA-C-O	-6.11	114.98	121.88
1	E	156	ILE	N-CA-C	-6.10	105.07	113.00
1	A	17	GLU	N-CA-C	-6.10	106.17	113.97
1	F	81	ILE	N-CA-C	-6.09	98.86	107.75
1	K	29	THR	N-CA-C	6.09	119.63	109.95
1	E	34	TYR	N-CA-C	-6.09	97.84	110.80
1	H	259	ALA	N-CA-C	-6.07	103.83	111.11
1	J	267	VAL	N-CA-C	6.07	117.31	108.58
1	K	232	THR	N-CA-C	-6.06	101.49	110.46
1	I	273	ILE	N-CA-C	6.05	117.19	108.48
1	L	36	GLY	CA-C-N	6.05	128.67	120.38
1	L	36	GLY	C-N-CA	6.05	128.67	120.38
1	D	256	ILE	CB-CA-C	-6.03	103.90	112.22
1	E	136	ALA	N-CA-C	6.03	118.46	108.99
1	G	261	GLU	N-CA-C	6.03	118.64	111.71
1	E	241	GLU	N-CA-C	-6.02	104.29	111.69
1	H	18	ALA	N-CA-C	-6.00	105.78	113.23
1	B	65	VAL	N-CA-C	-6.00	99.53	108.46
1	K	277	VAL	N-CA-C	6.00	113.78	108.63
1	E	176	GLY	N-CA-C	-5.99	105.19	115.61
1	I	82	GLU	N-CA-C	5.99	119.00	109.24
1	D	3	LEU	N-CA-C	5.98	119.69	110.42
1	E	40	GLU	CA-C-N	-5.98	113.97	122.94
1	E	40	GLU	C-N-CA	-5.98	113.97	122.94
1	E	112	ILE	N-CA-C	-5.98	104.68	110.42
1	C	26	VAL	N-CA-C	-5.94	100.91	108.93
1	L	183	ALA	N-CA-C	-5.94	101.57	110.24
1	K	41	SER	N-CA-C	-5.94	101.62	110.23
1	J	92	THR	N-CA-C	5.93	118.13	108.76
1	G	69	GLY	CA-C-N	5.92	127.25	119.84
1	G	69	GLY	C-N-CA	5.92	127.25	119.84
1	A	69	GLY	N-CA-C	5.91	124.40	112.34
1	J	64	VAL	N-CA-C	5.90	117.84	108.87
1	F	221	ALA	N-CA-C	5.89	123.34	110.80
1	E	69	GLY	N-CA-C	-5.88	100.34	112.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	179	ILE	CA-C-N	-5.88	113.72	119.78
1	K	179	ILE	C-N-CA	-5.88	113.72	119.78
1	F	255	LYS	N-CA-C	-5.88	104.87	111.28
1	I	95	ALA	N-CA-C	5.87	119.41	112.72
1	G	144	GLN	N-CA-C	5.87	123.30	110.80
1	J	83	SER	N-CA-C	5.87	123.29	110.80
1	B	136	ALA	N-CA-C	5.85	117.91	108.32
1	G	142	THR	N-CA-C	5.84	117.13	107.73
1	H	232	THR	N-CA-C	5.83	116.28	108.23
1	E	36	GLY	N-CA-C	-5.81	101.21	112.02
1	A	298	ARG	CA-C-N	5.81	129.35	121.05
1	A	298	ARG	C-N-CA	5.81	129.35	121.05
1	F	240	ASN	N-CA-C	-5.80	105.04	111.71
1	L	64	VAL	N-CA-C	5.80	116.94	108.53
1	K	92	THR	N-CA-C	5.79	118.33	108.02
1	K	67	GLY	N-CA-C	-5.78	105.85	112.79
1	H	237	GLU	N-CA-C	5.78	117.38	111.14
1	D	224	MET	N-CA-C	5.77	118.97	109.85
1	K	40	GLU	N-CA-C	5.77	119.81	111.56
1	F	194	TYR	N-CA-C	-5.74	100.43	109.50
1	C	15	LEU	N-CA-C	-5.74	105.16	111.82
1	C	148	MET	N-CA-C	5.72	120.00	113.19
1	D	11	VAL	N-CA-C	-5.72	104.35	110.36
1	D	220	ILE	N-CA-C	5.72	121.24	109.34
1	I	193	SER	N-CA-C	5.70	118.71	110.28
1	B	150	LYS	N-CA-C	-5.68	97.25	109.81
1	I	79	LEU	N-CA-C	-5.66	105.25	111.82
1	E	245	ASP	N-CA-C	5.66	117.25	111.14
1	E	220	ILE	N-CA-CB	-5.65	102.94	112.44
1	F	214	LEU	N-CA-C	-5.64	99.33	108.52
1	F	35	GLY	N-CA-C	5.63	126.53	113.18
1	F	296	SER	N-CA-C	-5.62	100.39	108.60
1	L	141	VAL	N-CA-C	5.62	121.03	109.34
1	J	226	LYS	N-CA-C	5.62	122.76	110.80
1	C	68	GLY	N-CA-C	5.60	126.46	113.18
1	K	8	ALA	N-CA-C	-5.60	105.27	111.71
1	G	236	THR	N-CA-C	-5.60	105.10	111.14
1	A	214	LEU	N-CA-C	-5.59	99.29	108.41
1	K	182	ILE	N-CA-C	5.58	116.63	108.53
1	F	167	VAL	N-CA-C	-5.58	104.85	113.16
1	L	277	VAL	CA-C-N	5.57	126.81	119.84
1	L	277	VAL	C-N-CA	5.57	126.81	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	40	GLU	N-CA-C	5.57	122.67	110.80
1	I	11	VAL	N-CA-C	5.56	115.76	110.42
1	H	82	GLU	N-CA-C	-5.56	103.15	110.43
1	G	15	LEU	N-CA-C	-5.54	105.34	111.71
1	G	21	TYR	N-CA-C	5.54	117.40	111.36
1	I	19	LEU	CA-C-N	-5.53	113.49	119.24
1	I	19	LEU	C-N-CA	-5.53	113.49	119.24
1	L	127	THR	N-CA-C	-5.51	101.59	110.14
1	B	92	THR	N-CA-C	5.51	118.54	107.41
1	I	272	ILE	N-CA-C	-5.51	99.30	107.51
1	E	236	THR	N-CA-C	5.50	117.99	111.33
1	H	294	LEU	N-CA-C	-5.50	101.51	110.20
1	K	175	LYS	N-CA-C	-5.48	104.74	111.75
1	C	64	VAL	N-CA-C	5.47	117.18	108.87
1	I	78	ARG	N-CA-C	5.46	117.09	111.03
1	I	163	THR	N-CA-C	-5.46	106.98	113.97
1	K	3	LEU	N-CA-C	-5.45	101.23	109.85
1	J	182	ILE	N-CA-C	5.45	115.70	107.80
1	I	41	SER	N-CA-C	-5.44	101.09	109.52
1	D	285	ILE	CB-CA-C	-5.44	102.37	111.29
1	J	269	SER	N-CA-C	5.43	118.44	109.85
1	E	256	ILE	CB-CA-C	-5.42	104.92	112.02
1	K	285	ILE	N-CA-C	5.41	116.28	111.90
1	J	80	SER	N-CA-C	5.41	122.32	110.80
1	B	148	MET	CA-C-N	-5.40	114.18	122.87
1	B	148	MET	C-N-CA	-5.40	114.18	122.87
1	H	45	LYS	N-CA-C	-5.40	104.63	111.11
1	A	298	ARG	N-CA-C	5.39	117.10	108.41
1	A	136	ALA	N-CA-C	5.39	115.66	108.38
1	A	92	THR	N-CA-C	5.39	116.23	107.23
1	I	120	GLY	N-CA-C	5.39	125.95	113.18
1	A	55	MET	N-CA-C	-5.38	105.31	111.07
1	A	50	ARG	N-CA-C	-5.37	105.42	111.28
1	E	60	ILE	N-CA-C	-5.34	100.62	108.85
1	G	162	VAL	N-CA-C	5.34	115.94	108.89
1	F	93	ASP	N-CA-C	-5.33	102.63	110.52
1	G	35	GLY	N-CA-C	-5.33	100.54	113.18
1	K	199	ASP	N-CA-C	-5.33	105.38	111.14
1	A	3	LEU	N-CA-C	-5.33	98.15	107.20
1	K	232	THR	CA-C-N	-5.32	113.52	122.25
1	K	232	THR	C-N-CA	-5.32	113.52	122.25
1	C	273	ILE	N-CA-C	5.32	117.29	108.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	160	GLY	N-CA-C	5.32	125.79	113.18
1	H	281	VAL	N-CA-C	5.31	116.04	110.62
1	D	210	LYS	N-CA-C	-5.31	103.91	111.24
1	E	137	LYS	N-CA-C	-5.29	101.71	109.81
1	A	300	ARG	N-CA-C	5.29	122.07	110.80
1	I	247	THR	N-CA-C	-5.29	106.67	113.23
1	B	34	TYR	CA-C-N	-5.29	113.75	122.05
1	B	34	TYR	C-N-CA	-5.29	113.75	122.05
1	B	69	GLY	N-CA-C	5.28	123.11	112.34
1	K	43	GLU	N-CA-C	-5.28	106.97	113.41
1	L	250	GLY	N-CA-C	5.28	120.87	111.73
1	B	64	VAL	N-CA-C	5.26	116.87	108.87
1	F	289	SER	N-CA-C	5.26	122.00	110.80
1	B	80	SER	CA-C-N	5.26	130.03	123.14
1	B	80	SER	C-N-CA	5.26	130.03	123.14
1	K	291	VAL	N-CA-C	-5.25	104.69	112.04
1	A	10	GLN	N-CA-C	-5.25	105.25	110.97
1	B	246	GLY	N-CA-C	-5.24	107.88	115.27
1	D	25	PHE	N-CA-C	5.24	120.33	113.30
1	H	221	ALA	N-CA-C	5.24	121.96	110.80
1	L	273	ILE	N-CA-C	5.23	116.26	108.46
1	A	234	LEU	N-CA-C	5.23	118.01	109.59
1	A	72	ILE	CB-CA-C	-5.23	105.00	112.22
1	K	219	ASN	N-CA-C	5.23	119.81	113.38
1	G	85	PHE	N-CA-CB	-5.22	101.66	110.49
1	A	64	VAL	N-CA-C	5.20	115.75	108.89
1	I	289	SER	CA-C-N	-5.20	111.23	121.41
1	I	289	SER	C-N-CA	-5.20	111.23	121.41
1	E	5	ARG	CA-C-O	5.19	127.93	120.51
1	B	220	ILE	N-CA-CB	-5.18	102.41	110.96
1	E	194	TYR	N-CA-C	-5.18	99.89	108.75
1	E	244	ALA	CA-C-N	5.18	127.48	120.44
1	E	244	ALA	C-N-CA	5.18	127.48	120.44
1	J	136	ALA	N-CA-C	5.18	116.94	109.07
1	F	127	THR	N-CA-C	-5.17	102.51	109.95
1	K	206	ALA	N-CA-C	-5.17	105.82	111.82
1	F	160	GLY	N-CA-C	5.17	125.42	113.18
1	D	37	ASN	N-CA-C	-5.15	105.10	111.33
1	A	43	GLU	N-CA-C	5.15	117.63	111.71
1	J	84	HIS	N-CA-C	5.15	116.29	107.28
1	H	234	LEU	N-CA-C	5.14	117.70	110.14
1	B	168	GLY	N-CA-C	-5.14	106.54	112.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	195	ASN	N-CA-C	-5.13	101.34	109.96
1	E	93	ASP	N-CA-C	-5.13	102.42	110.17
1	I	139	LEU	N-CA-C	5.13	117.09	108.73
1	J	16	SER	N-CA-C	-5.12	104.77	111.02
1	C	120	GLY	N-CA-C	5.12	122.37	115.00
1	G	224	MET	N-CA-C	5.11	117.78	109.24
1	H	65	VAL	N-CA-C	-5.11	100.53	108.86
1	H	160	GLY	N-CA-C	5.11	119.57	112.57
1	A	297	ASN	N-CA-C	-5.11	104.67	111.87
1	J	3	LEU	N-CA-C	-5.10	99.93	110.80
1	C	252	MET	N-CA-C	-5.09	107.02	113.18
1	E	57	ALA	N-CA-C	-5.09	105.91	111.82
1	K	249	TYR	N-CA-C	5.08	116.72	109.14
1	A	15	LEU	N-CA-C	-5.08	105.63	111.07
1	K	24	ARG	N-CA-C	5.07	117.47	111.33
1	L	191	GLY	N-CA-C	5.07	125.19	113.18
1	A	176	GLY	N-CA-C	-5.06	107.68	115.73
1	B	258	CYS	CB-CA-C	-5.06	103.10	110.95
1	I	226	LYS	N-CA-C	-5.06	106.80	112.87
1	K	183	ALA	CA-C-N	5.06	126.17	119.84
1	K	183	ALA	C-N-CA	5.06	126.17	119.84
1	J	32	ILE	N-CA-C	5.05	115.13	107.80
1	L	68	GLY	O-C-N	5.05	124.68	121.85
1	E	26	VAL	N-CA-C	5.05	119.83	109.34
1	E	85	PHE	N-CA-C	5.05	117.64	109.06
1	I	67	GLY	N-CA-C	-5.04	101.23	113.18
1	F	161	GLU	N-CA-C	-5.04	100.69	108.90
1	A	66	HIS	N-CA-C	5.03	118.22	110.42
1	J	127	THR	N-CA-C	-5.03	102.44	109.69
1	L	37	ASN	CA-C-N	5.03	131.15	121.54
1	L	37	ASN	C-N-CA	5.03	131.15	121.54
1	H	85	PHE	CB-CA-C	-5.03	101.50	113.02
1	I	167	VAL	N-CA-C	-5.03	105.67	113.16
1	L	38	ALA	N-CA-C	5.03	121.50	110.80
1	B	59	GLY	N-CA-C	5.02	121.74	115.21
1	L	154	ILE	N-CA-C	-5.01	100.53	107.80
1	L	267	VAL	N-CA-C	-5.01	101.25	108.87
1	I	97	MET	N-CA-C	-5.01	105.28	111.40
1	H	60	ILE	N-CA-C	5.01	114.78	107.37
1	H	127	THR	N-CA-C	-5.01	102.74	109.95

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2159	0	2259	171	0
1	B	2177	0	2265	198	0
1	C	2201	0	2302	150	0
1	D	2170	0	2272	114	0
1	E	2106	0	2196	162	0
1	F	2131	0	2213	199	0
1	G	2186	0	2278	204	0
1	H	2173	0	2270	242	0
1	I	2110	0	2195	239	0
1	J	2015	0	2071	286	0
1	K	1918	0	1917	277	0
1	L	2163	0	2265	229	0
2	A	13	0	9	0	0
2	B	13	0	9	1	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
3	I	27	0	12	0	0
3	J	27	0	12	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	L	27	0	12	4	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	2298	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 44.

All (2298) 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:B:32:ILE:HD11	1:B:55:MET:HE1	1.13	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:H:97:MET:HE1	1:H:195:ASN:HB2	1.31	1.10
1:B:35:GLY:HA2	1:B:39:MET:HE3	1.32	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:195:ASN:ND2	2:H:1299:NLG:H8C3	1.67	1.09
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:C:172:MET:HG2	1:D:172:MET:HE2	1.33	1.07
1:G:223:LEU:HD13	1:G:256:ILE:HD11	1.34	1.07
1:K:260:LEU:HD23	1:K:295:ILE:HD11	1.35	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:K:129:LYS:HD2	1:K:187:VAL:CG2	1.84	1.06
1:L:84:HIS:NE2	1:L:91:VAL:HG21	1.70	1.06
1:I:273:ILE:CD1	1:I:284:GLU:HG3	1.85	1.06
1:H:92:THR:HG21	1:H:97:MET:HE3	1.30	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: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:H:92:THR:CG2	1:H:97:MET:HE3	1.89	1.00
1:J:282:LEU:HD23	1:K:12:ALA:CA	1.90	1.00
1:G:86:ILE:CD1	1:G:91:VAL:HG21	1.92	1.00
1:G:253:LEU:HB2	1:G:254:PRO:HD3	1.41	1.00
1:B:54:LEU:HD21	1:C:15:LEU:HD23	1.44	1.00
1:C:97:MET:HE1	1:C:195:ASN:HB2	1.39	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:A:22:ILE:HG23	1:A:58:VAL:HG13	1.41	0.99
1:G:39:MET:HA	1:G:39:MET:HE3	1.40	0.99
1:H:92:THR:HG21	1:H:97:MET:CE	1.92	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:96:THR:O	1:H:100:VAL:HG23	1.62	0.99
1:B:97:MET:HE1	1:B:195:ASN:N	1.77	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
1:J:219:ASN:ND2	1:J:220:ILE:HG13	1.78	0.97
1:F:97:MET:HE1	1:F:195:ASN:HB2	1.46	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:K:109:ASN:C	1:K:109:ASN:HD22	1.72	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:G:32:ILE:HD11	1:G:55:MET:HE1	1.47	0.96
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:L:30:LEU:HD13	1:L:215:MET:HE1	1.49	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:E:97:MET:HE1	1:E:195:ASN:N	1.81	0.94
1:H:232:THR:HG22	1:H:233:GLY:N	1.83	0.94
1:H:39:MET:HE1	1:H:217:LEU:CG	1.98	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	0.93
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:37:ASN:HD21	1:K:40:GLU:HG2	1.28	0.91
1:K:72:ILE:HD11	1:K:104:LEU:HG	1.53	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:36:GLY:H	1:J:68:GLY:HA3	1.35	0.90
1:J:282:LEU:HD23	1:K:12:ALA:CB	2.01	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:I:223:LEU:C	1:I:223:LEU:HD12	1.97	0.89
1:H:33:LYS:HB3	1:H:216:LEU:HD12	1.54	0.89
1:J:35:GLY:O	1:J:39:MET:HE3	1.72	0.89
1:K:178:PHE:O	1:K:180:PRO:HD3	1.73	0.89
1:B:35:GLY:CA	1:B:39:MET:HE3	2.03	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:I:55:MET:HE3	1:I:285:ILE:HD11	1.54	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: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:97:MET:HE1	1:A:195:ASN:HB2	1.55	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:103:VAL:HG13	1:K:107:GLN:CD	2.01	0.86
1:F:89:MET:HE1	1:F:139:LEU:HD23	1.56	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:B:32:ILE:CD1	1:B:55:MET:HE1	2.03	0.86
1:J:219:ASN:C	1:J:219:ASN:HD22	1.77	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
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:H:39:MET:HE1	1:H:217:LEU:CD2	2.05	0.85
1:K:271:HIS:ND1	1:K:284:GLU:HG2	1.91	0.85
1:D:253:LEU:HB3	1:D:254:PRO:HD3	1.58	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:I:55:MET:HE1	1:I:215:MET:HE1	1.58	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:39:MET:HE3	1:H:275:GLY:HA3	1.57	0.84
1:H:21:TYR:O	1:H:24:ARG:HG2	1.77	0.84
1:H:23:ARG:HG3	1:H:23:ARG:HH11	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:G:172:MET:HE3	1:H:172:MET:HG2	1.58	0.83
1:H:39:MET:HE1	1:H:217:LEU:HG	1.58	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:I:96:THR:O	1:I:100:VAL:HG23	1.77	0.83
1:F:89:MET:HE3	1:F:156:ILE:HG21	1.60	0.82
1:G:211:ALA:O	1:G:267:VAL:HG13	1.79	0.82
1:I:102:MET:HE1	1:J:75:LEU:HD22	1.62	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:H	1:L:143:ARG:HD2	1.43	0.82
1:G:118:ARG:HH11	1:G:118:ARG:CA	1.92	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
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:H:97:MET:HA	1:H:97:MET:HE2	1.62	0.81
1:J:30:LEU:HD12	1:J:60:ILE:CG2	2.10	0.81
1:J:223:LEU:HD21	1:J:248:ILE:HD11	1.60	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: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:K:92:THR:HG21	1:K:97:MET:HE3	1.62	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: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:H:12:ALA:HB3	1:L:50:ARG:NH2	1.96	0.80
1:K:71:GLN:HB3	1:K:107:GLN:HE21	1.41	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:HH11	1:J:118:ARG:CB	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:J:178:PHE:O	1:J:180:PRO:HD3	1.83	0.79
1:J:252:MET:HE2	1:J:272:ILE:HD13	1.64	0.79
1:K:34:TYR:HE1	1:K:37:ASN:HB2	1.45	0.79
1:L:54:LEU:CD2	1:L:282:LEU:HD21	2.12	0.79
1:L:140:THR:HG22	1:L:153:ILE:HD13	1.64	0.79
1:C:221:ALA:CA	1:C:274:ASP:HB2	2.11	0.79
1:D:3:LEU:HD23	1:D:3:LEU:N	1.98	0.79
1:D:299:LYS:O	1:D:299:LYS:HG2	1.83	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:39:MET:HE1	1:H:217:LEU:HD23	1.64	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: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:226:LYS:C	1:G:228:GLY:H	1.92	0.77
1:G:66:HIS:O	1:G:184:PRO:HD3	1.85	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:23:ARG:HG2	1:A:23:ARG:HH11	1.48	0.77
1:A:234:LEU:CD2	1:A:239:VAL:HG23	2.15	0.77
1:G:5:ARG:NH1	1:I:291:VAL:HG22	1.99	0.77
1:G:39:MET:HE1	1:G:44:LEU:HD23	1.64	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:D:252:MET:HE3	1:D:255:LYS:HB3	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
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:HH11	1:J:118:ARG:CG	1.98	0.76
1:F:89:MET:HE1	1:F:139:LEU:CD2	2.15	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:K:109:ASN:C	1:K:109:ASN:ND2	2.44	0.75
1:K:273:ILE:HD11	1:K:284:GLU:CD	2.11	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:285:ILE:O	1:H:285:ILE:HG12	1.85	0.75
1:L:229:GLN:HA	1:L:229:GLN:HE21	1.50	0.75
1:A:36:GLY:C	1:A:38:ALA:H	1.93	0.74
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:B:32:ILE:HD11	1:B:55:MET:CE	2.07	0.74
1:E:97:MET:HE1	1:E:195:ASN:H	1.52	0.74
1:G:36:GLY:C	1:G:39:MET:HB3	2.12	0.74
1:G:72:ILE:HD12	1:G:90:ARG:HH21	1.52	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:D:219:ASN:HD22	1:D:219:ASN:C	1.93	0.74
1:F:218:THR:HG23	1:F:220:ILE:N	1.99	0.74
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:A:97:MET:HE1	1:A:195:ASN:CB	2.19	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:G:172:MET:CE	1:H:172:MET:HE2	2.18	0.73
1:G:172:MET:HE2	1:H:172:MET:HE2	1.69	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:78:ARG:HG2	1:J:79:LEU:HD11	1.71	0.73
1:D:252:MET:HE1	1:D:255:LYS:HD2	1.70	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: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: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:G:39:MET:HE1	1:G:44:LEU:CD2	2.18	0.72
1:L:82:GLU:CG	1:L:83:SER:H	2.01	0.72
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:54:LEU:HD11	1:F:15:LEU:HD12	1.72	0.72
1:D:248:ILE:HG21	1:D:256:ILE:CD1	2.20	0.72
1:F:167:VAL:HG23	1:F:171:ASN:HD21	1.53	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:E:39:MET:HE1	1:E:68:GLY:HA2	1.71	0.72
1:F:3:LEU:HD11	1:F:11:VAL:HB	1.71	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:C:223:LEU:C	1:C:223:LEU:HD12	2.15	0.71
1:G:55:MET:HE3	1:G:285:ILE:HD11	1.73	0.71
1:I:55:MET:HE2	1:I:285:ILE:HD11	1.72	0.71
1:J:282:LEU:CD2	1:K:12:ALA:CA	2.53	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:G:252:MET:HE1	1:G:272:ILE:CD1	2.20	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: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:A:86:ILE:HD12	1:A:156:ILE:HD11	1.73	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
1:L:82:GLU:HG2	1:L:83:SER:H	1.55	0.70
1:L:279:ASN:O	1:L:283:LEU:HG	1.92	0.70
1:A:92:THR:HG21	1:A:97:MET:HE2	1.72	0.70
1:K:172:MET:HE1	1:L:173:LEU:HA	1.74	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:C:71:GLN:CD	1:C:71:GLN:H	1.99	0.69
1:G:65:VAL:HG21	1:G:202:ALA:HA	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:N	1:G:85:PHE:CD1	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:173:LEU:HD23	1:F:172:MET:HE1	1.75	0.69
1:E:287:THR:CG2	1:E:288:ASP:N	2.55	0.69
1:A:243:ILE:HG12	1:A:248:ILE:HD12	1.73	0.69
1:B:34:TYR:CD2	1:B:39:MET:HE2	2.27	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:I:29:THR:HG22	1:I:61:ASN:HB2	1.74	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:A:36:GLY:C	1:A:38:ALA:N	2.49	0.68
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
1:K:100:VAL:HG11	1:K:195:ASN:ND2	2.07	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:F:219:ASN:C	1:F:219:ASN:HD22	2.02	0.68
1:I:93:ASP:CG	1:I:96:THR:HG23	2.17	0.68
1:A:30:LEU:HD13	1:A:55:MET:HE3	1.74	0.68
1:E:55:MET:HE3	1:E:285:ILE:HD11	1.75	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:35:GLY:HA2	1:E:39:MET:HG3	1.74	0.68
1:G:8:ALA:HB2	1:I:287:THR:CG2	2.24	0.68
1:G:86:ILE:CG2	1:G:87:ASP:H	2.07	0.68
1:J:15:LEU:CD1	1:K:15:LEU:HD21	2.22	0.68
1:J:282:LEU:O	1:J:286:PHE:HD1	1.77	0.68
1:L:68:GLY:CA	1:L:104:LEU:HD21	2.23	0.68
1:I:176:GLY:HA3	1:J:172:MET:HE1	1.74	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:2:THR:HG22	1:J:3:LEU:N	2.09	0.67
1:J:188:GLY:HA3	1:J:192:GLU:OE2	1.94	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:19:LEU:HD23	1:E:22:ILE:HD11	1.77	0.67
1:E:50:ARG:HB2	1:E:119:HIS:ND1	2.10	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
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:D:30:LEU:HD12	1:D:55:MET:HE3	1.75	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:9:ALA:HA	1:I:283:LEU:HD21	1.75	0.67
1:G:56:LYS:HA	1:G:60:ILE:O	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:68:GLY:O	1:B:70:PRO:HD2	1.95	0.66
1:G:118:ARG:HH11	1:G:118:ARG:HG2	1.60	0.66
1:J:219:ASN:ND2	1:J:219:ASN:C	2.49	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:HG3	1:H:23:ARG:NH1	2.03	0.66
1:A:30:LEU:CD1	1:A:55:MET:HE3	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:H	1:I:5:ARG:HD3	1.59	0.66
1:J:30:LEU:HD22	1:J:215:MET:CE	2.24	0.66
1:J:230:VAL:HG11	1:J:292:GLY:HA2	1.77	0.66
1:L:84:HIS:CE1	1:L:91:VAL:HG11	2.31	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: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: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
1:J:54:LEU:HD23	1:J:282:LEU:CD1	2.21	0.66
1:J:117:ASN:HA	1:J:121:GLY:O	1.95	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: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: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:J:31:VAL:HG21	1:J:206:ALA:HA	1.78	0.65
1:K:232:THR:CG2	1:K:294:LEU:HB3	2.26	0.65
1:B:50:ARG:CZ	1:C:12:ALA:HB1	2.26	0.65
1:B:129:LYS:HD3	1:B:187:VAL:CG1	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:213:LYS:HB2	1:B:269:SER:OG	1.97	0.65
1:E:37:ASN:C	1:E:219:ASN:HD21	2.04	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:A:51:ASP:CG	1:A:282:LEU:HG	2.22	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
1:H:19:LEU:O	1:H:23:ARG:CG	2.44	0.64
1:H:112:ILE:O	1:H:116:ILE:HG13	1.96	0.64
1:L:224:MET:HA	1:L:229:GLN:O	1.97	0.64
1:E:58:VAL:O	1:E:58:VAL:HG12	1.95	0.64
1:F:30:LEU:HD13	1:F:215:MET:HE2	1.78	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:J:97:MET:HE1	1:J:195:ASN:ND2	2.12	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:24:ARG:HD2	1:K:25:PHE:CE2	2.32	0.64
1:K:127:THR:HG22	1:K:183:ALA:CB	2.20	0.64
1:G:71:GLN:HG3	1:G:108:VAL:HG21	1.79	0.64
1:B:199:ASP:HB3	1:B:258:CYS:SG	2.38	0.64
1:I:224:MET:HE2	1:I:228:GLY:HA2	1.79	0.64
1:B:58:VAL:HG13	1:B:58:VAL:O	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:287:THR:CG2	1:B:288:ASP:H	2.10	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:A:221:ALA:HB3	1:A:224:MET:HE3	1.78	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:L:30:LEU:HD13	1:L:215:MET:CE	2.27	0.64
1:C:220:ILE:HG13	1:C:220:ILE:O	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:O	1:I:58:VAL:HG12	1.98	0.64
1:K:76:LEU:CD2	1:K:99:VAL:HG11	2.27	0.64
1:K:179:ILE:O	1:K:179:ILE:HG22	1.97	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:L:252:MET:HE3	1:L:255:LYS:HD2	1.80	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
1:B:97:MET:HE1	1:B:194:TYR:C	2.23	0.63
1:B:252:MET:HE3	1:B:255:LYS:HB3	1.78	0.63
1:J:15:LEU:HB2	1:K:15:LEU:HD21	1.78	0.63
1:K:33:LYS:HA	1:K:65:VAL:O	1.98	0.63
1:K:196:ILE:CG2	1:K:200:LEU:CD2	2.76	0.63
1:A:101:GLU:CG	1:A:185:ILE:HD13	2.28	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: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:F:252:MET:HE3	1:F:255:LYS:HB3	1.79	0.63
1:I:38:ALA:HB3	1:I:219:ASN:OD1	1.98	0.63
1:I:273:ILE:HD13	1:I:284:GLU:CG	2.25	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:ARG:HG2	1:A:23:ARG:NH1	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:22:ILE:HG21	1:F:58:VAL:HG13	1.80	0.63
1:F:142:THR:CG2	1:F:151:PRO:HB3	2.29	0.63
1:H:196:ILE:HG22	1:H:197:ASN:N	2.13	0.63
1:I:92:THR:HG22	1:I:96:THR:OG1	1.99	0.63
1:I:117:ASN:HD21	1:I:123:ALA:HB3	1.62	0.63
1:L:33:LYS:HA	1:L:65:VAL:O	1.99	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
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:A:285:ILE:C	1:A:287:THR:H	2.08	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:252:MET:HE1	1:F:272:ILE:HG21	1.82	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:18:ALA:O	1:K:22:ILE:HG13	2.00	0.62
1:K:107:GLN:HG3	1:K:108:VAL:N	2.15	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: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:25:PHE:HD2	1:J:212:GLU:HG2	1.64	0.62
1:J:137:LYS:CG	1:J:138:LYS:H	2.13	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:C:92:THR:HG21	1:C:97:MET:HE2	1.81	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:J:33:LYS:HD3	1:J:33:LYS:C	2.25	0.61
1:E:251:GLY:HA3	3:E:1299:ADP:O2A	1.99	0.61
1:H:69:GLY:H	1:H:70:PRO:HD3	1.61	0.61
1:I:30:LEU:HD22	1:I:213:LYS:HB3	1.82	0.61
1:K:72:ILE:HA	1:K:103:VAL:HG11	1.81	0.61
1:K:271:HIS:CD2	1:K:294:LEU:HD12	2.35	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:I:100:VAL:HG11	1:I:195:ASN:OD1	2.01	0.61
1:J:34:TYR:CD2	1:J:35:GLY:N	2.68	0.61
1:J:248:ILE:HD13	1:J:256:ILE:CD1	2.30	0.61
1:I:23:ARG:HG2	1:I:23:ARG:HH11	1.65	0.61
1:J:30:LEU:HD12	1:J:60:ILE:HG21	1.80	0.61
1:L:252:MET:O	1:L:252:MET:HG3	1.99	0.61
1:H:19:LEU:HD21	1:L:53:VAL:HG11	1.81	0.61
1:D:219:ASN:C	1:D:219:ASN:ND2	2.56	0.61
1:J:209:LEU:O	1:J:210:LYS:C	2.42	0.61
1:L:73:GLY:HA2	1:L:76:LEU:HD12	1.83	0.61
1:G:156:ILE:HG22	1:G:156:ILE:O	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:B:32:ILE:HG12	1:B:215:MET:HE3	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:54:LEU:O	1:H:58:VAL:HG23	2.00	0.61
1:H:217:LEU:HG	1:H:275:GLY:HA3	1.83	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:243:ILE:HD13	1:D:243:ILE:C	2.26	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:B:294:LEU:HD23	1:B:294:LEU:C	2.26	0.60
1:D:225:ASP:OD1	1:D:231:LEU:HD21	2.01	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:G:148:MET:HE1	1:G:152:GLU:HB3	1.83	0.60
1:L:143:ARG:HD2	1:L:143:ARG:N	2.14	0.60
1:B:167:VAL:HG23	1:B:171:ASN:ND2	2.15	0.60
1:D:30:LEU:HD12	1:D:55:MET:CE	2.31	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
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:E:215:MET:HE3	1:E:281:VAL:HG22	1.84	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:HH11	1:H:90:ARG:HG3	1.66	0.60
1:J:38:ALA:C	1:J:40:GLU:H	2.10	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:D:271:HIS:CE1	1:D:284:GLU:HG2	2.37	0.60
1:B:175:LYS:HG3	1:B:175:LYS:O	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:89:MET:HE1	1:L:200:LEU:CD1	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:55:MET:HE2	1:C:285:ILE:HD13	1.84	0.59
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:37:ASN:O	1:J:40:GLU:CG	2.50	0.59
1:J:248:ILE:HG22	1:J:253:LEU:HD23	1.84	0.59
1:A:22:ILE:CG2	1:A:58:VAL:HG13	2.23	0.59
1:A:101:GLU:HA	1:A:185:ILE:HD11	1.84	0.59
1:D:253:LEU:CB	1:D:254:PRO:HD3	2.32	0.59
1:I:32:ILE:HG12	1:I:215:MET:HE3	1.84	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:I:30:LEU:HD12	1:I:55:MET:HE2	1.83	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
1:C:273:ILE:HG12	1:C:274:ASP:N	2.17	0.59
1:C:291:VAL:HG23	1:C:291:VAL:O	2.03	0.59
1:H:92:THR:HG22	1:H:97:MET:HE3	1.82	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:B:252:MET:HE3	1:B:255:LYS:CB	2.32	0.59
1:C:101:GLU:HG3	1:C:185:ILE:HD13	1.84	0.59
1:C:297:ASN:O	1:C:298:ARG:HB2	2.02	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:86:ILE:HG23	1:I:86:ILE:O	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:248:ILE:HG21	1:D:256:ILE:HD11	1.85	0.59
1:D:252:MET:CE	1:D:255:LYS:HB3	2.32	0.59
1:E:10:GLN:HG2	1:E:11:VAL:H	1.65	0.59
1:D:223:LEU:HD23	1:D:223:LEU:C	2.27	0.59
1:F:271:HIS:ND1	1:F:284:GLU:CG	2.65	0.59
1:H:39:MET:CE	1:H:217:LEU:HG	2.32	0.59
1:I:262:ALA:O	1:I:267:VAL:HB	2.03	0.59
1:J:55:MET:HE2	1:J:60:ILE:HG21	1.83	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: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:75:LEU:HD22	1:L:102:MET:SD	2.43	0.58
1:K:97:MET:CE	1:K:195:ASN:HB2	2.33	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:H:34:TYR:HD2	1:H:35:GLY:H	1.50	0.58
1:H:92:THR:CG2	1:H:97:MET:CE	2.66	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
1:J:3:LEU:CD2	1:K:21:TYR:CE2	2.83	0.58
1:K:227:GLN:O	1:K:228:GLY:C	2.46	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:F:244:ALA:C	1:F:246:GLY:N	2.55	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: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:58:VAL:O	1:E:58:VAL:CG1	2.50	0.58
1:E:66:HIS:O	1:E:184:PRO:HD3	2.02	0.58
1:E:127:THR:HG22	1:E:183:ALA:HB3	1.86	0.58
1:H:232:THR:CG2	1:H:294:LEU:HB3	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:72:ILE:HD11	1:B:104:LEU:HG	1.85	0.58
1:D:252:MET:HE1	1:D:272:ILE:HD13	1.85	0.58
1:D:291:VAL:O	1:D:291:VAL:HG12	2.03	0.58
1:F:30:LEU:HD12	1:F:55:MET:CE	2.34	0.58
1:G:2:THR:HG22	1:G:2:THR:O	2.03	0.58
1:H:287:THR:HG23	1:L:3:LEU:HB3	1.83	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:L:38:ALA:C	1:L:40:GLU:H	2.10	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:F:207:GLU:CD	1:F:265:GLY:HA3	2.29	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: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:I:102:MET:HE1	1:J:75:LEU:CD2	2.34	0.57
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
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:H	1:F:219:ASN:ND2	2.02	0.57
1:G:252:MET:HE1	1:G:272:ILE:HD13	1.85	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:93:ASP:OD1	1:E:93:ASP:N	2.36	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:H:19:LEU:HD21	1:L:53:VAL:CG1	2.33	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:H:10:GLN:HG3	1:H:11:VAL:N	2.17	0.57
1:I:56:LYS:CE	1:I:177:ASP:OD1	2.52	0.57
1:I:117:ASN:ND2	1:I:123:ALA:N	2.45	0.57
1:F:11:VAL:HG13	1:F:15:LEU:HD11	1.87	0.57
1:H:97:MET:CE	1:H:97:MET:HA	2.32	0.57
1:J:30:LEU:HD22	1:J:215:MET:HE2	1.84	0.57
1:J:162:VAL:HB	1:J:204:LYS:HG3	1.87	0.57
1:J:225:ASP:C	1:J:225:ASP:OD1	2.48	0.57
1:F:11:VAL:HG13	1:F:15:LEU:HG	1.87	0.56
1:H:218:THR:HG23	1:H:220:ILE:O	2.05	0.56
1:I:107:GLN:NE2	1:J:102:MET:HE1	2.19	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:A:245:ASP:C	1:A:245:ASP:OD1	2.47	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:I:195:ASN:C	1:I:196:ILE:HG13	2.30	0.56
1:J:19:LEU:HD22	1:K:54:LEU:HD13	1.88	0.56
1:B:34:TYR:CD1	1:B:48:PHE:CG	2.93	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:C:213:LYS:HD3	1:C:271:HIS:NE2	2.20	0.56
1:D:252:MET:CE	1:D:255:LYS:HD2	2.34	0.56
1:D:271:HIS:N	1:D:271:HIS:CD2	2.73	0.56
1:F:200:LEU:HD23	1:F:258:CYS:SG	2.45	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:118:ARG:NH1	1:G:118:ARG:HG2	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:I:223:LEU:C	1:I:223:LEU:CD1	2.71	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:35:GLY:CA	1:E:39:MET:HG3	2.36	0.56
1:E:167:VAL:HG12	1:E:171:ASN:HD21	1.66	0.56
1:G:89:MET:HB3	2:G:1301:NLG:C8	2.34	0.56
1:J:37:ASN:O	1:J:40:GLU:N	2.36	0.56
1:J:54:LEU:CD2	1:J:282:LEU:CD1	2.83	0.56
1:J:273:ILE:HG22	1:J:274:ASP:N	2.21	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:B:34:TYR:HD1	1:B:48:PHE:CD1	2.22	0.56
1:B:253:LEU:HB2	1:B:254:PRO:HD3	1.86	0.56
1:C:252:MET:HE3	1:C:255:LYS:HB3	1.88	0.56
1:E:55:MET:HE3	1:E:285:ILE:CD1	2.34	0.56
1:G:72:ILE:HG21	1:G:100:VAL:HG22	1.87	0.56
1:A:294:LEU:C	1:A:294:LEU:HD12	2.30	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
1:G:86:ILE:CD1	1:G:91:VAL:CG2	2.76	0.56
1:I:79:LEU:HD22	1:J:78:ARG:NE	2.21	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:K:34:TYR:CZ	1:K:37:ASN:HB2	2.40	0.56
1:L:237:GLU:CD	1:L:237:GLU:H	2.13	0.56
1:A:234:LEU:O	1:A:295:ILE:HA	2.06	0.56
1:A:235:SER:OG	1:A:238:GLN:HG3	2.06	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:G:173:LEU:HA	1:H:172:MET:HE1	1.88	0.56
1:H:70:PRO:CD	1:H:71:GLN:OE1	2.52	0.56
1:L:131:ALA:HB3	1:L:169:LEU:HD22	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:136:ALA:O	1:L:188:GLY:HA2	2.06	0.56
1:L:252:MET:HE3	1:L:255:LYS:HB3	1.88	0.56
1:D:212:GLU:O	1:D:268:THR:HB	2.05	0.56
1:H:7:ASP:O	1:H:11:VAL:HG23	2.06	0.56
1:I:92:THR:HG22	1:I:96:THR:HG1	1.70	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:37:ASN:O	1:I:249:TYR:CE2	2.59	0.55
1:C:44:LEU:HD21	1:C:276:ARG:HA	1.87	0.55
1:F:30:LEU:HD12	1:F:55:MET:HE2	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:K:30:LEU:CD2	1:K:213:LYS:HB2	2.37	0.55
1:K:162:VAL:HB	1:K:204:LYS:HG3	1.86	0.55
1:L:220:ILE:HG23	1:L:222:GLY:H	1.71	0.55
1:G:39:MET:HE3	1:G:44:LEU:HD23	1.86	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: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:73:GLY:O	1:F:77:LYS:HD3	2.06	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:G:39:MET:HA	1:G:39:MET:CE	2.25	0.55
1:H:18:ALA:C	1:H:22:ILE:HD12	2.31	0.55
1:I:257:ARG:O	1:I:261:GLU:CG	2.54	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
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:B:34:TYR:HD2	1:B:39:MET:HE2	1.68	0.55
1:B:144:GLN:CD	1:B:149:THR:HG21	2.30	0.55
1:C:58:VAL:HG13	1:C:58:VAL:O	2.07	0.55
1:C:230:VAL:CG1	1:C:292:GLY:HA2	2.34	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:21:TYR:HD1	1:K:21:TYR:H	1.55	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:D:35:GLY:C	1:D:37:ASN:H	2.14	0.55
1:E:291:VAL:CG2	1:E:292:GLY:N	2.70	0.55
1:K:126:LEU:O	1:K:182:ILE:HA	2.07	0.55
1:G:11:VAL:HG12	1:I:286:PHE:CD2	2.41	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: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:89:MET:HE2	1:I:200:LEU:HD11	1.89	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:K:213:LYS:HZ1	1:K:271:HIS:CE1	2.25	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:I:209:LEU:O	1:I:210:LYS:C	2.49	0.54
1:A:128:GLY:HA3	1:A:185:ILE:O	2.06	0.54
1:C:16:SER:HA	1:C:19:LEU:HD12	1.89	0.54
1:C:146:PRO:HD2	1:C:149:THR:HB	1.89	0.54
1:F:75:LEU:O	1:F:76:LEU:C	2.49	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:C:215:MET:HE2	1:C:284:GLU:HB2	1.89	0.54
1:H:196:ILE:HG22	1:H:197:ASN:H	1.71	0.54
1:J:2:THR:CG2	1:J:3:LEU:H	2.16	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:154:ILE:CG2	1:B:155:ASP:N	2.69	0.54
1:G:15:LEU:CB	1:I:54:LEU:HD21	2.37	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:A:32:ILE:HG12	1:A:215:MET:HE3	1.90	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:37:ASN:HB2	1:B:219:ASN:CG	2.31	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:11:VAL:HG12	1:I:286:PHE:CE2	2.43	0.54
1:G:195:ASN:C	1:G:196:ILE:HG13	2.32	0.54
1:K:213:LYS:NZ	1:K:271:HIS:CE1	2.75	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: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: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:172:MET:HE1	1:J:178:PHE:HE1	1.71	0.54
1:J:25:PHE:CD2	1:J:212:GLU:HG2	2.43	0.54
1:J:86:ILE:HG22	1:J:89:MET:O	2.08	0.54
1:J:134:ILE:HD13	1:J:201:VAL:HG11	1.89	0.54
1:K:82:GLU:HA	1:K:82:GLU:OE2	2.07	0.54
1:K:296:SER:O	1:K:297:ASN:CB	2.54	0.54
1:L:30:LEU:HD22	1:L:213:LYS:HB3	1.89	0.54
1:L:162:VAL:HG11	1:L:204:LYS:HB3	1.90	0.54
1:B:35:GLY:HA2	1:B:39:MET:CE	2.22	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:G:32:ILE:HD11	1:G:55:MET:CE	2.30	0.54
1:H:5:ARG:HG3	1:H:6:ASP:N	2.22	0.54
1:H:220:ILE:HG13	1:H:224:MET:HE2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:23:ARG:NH2	1:L:120:GLY:O	2.41	0.53
1:I:69:GLY:O	1:I:72:ILE:HB	2.08	0.53
1:I:87:ASP:OD1	1:I:253:LEU:HD13	2.08	0.53
1:J:7:ASP:O	1:J:10:GLN:HB2	2.08	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: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:J:296:SER:C	1:J:298:ARG:N	2.62	0.53
1:K:285:ILE:HG13	1:K:286:PHE:N	2.24	0.53
1:F:252:MET:HE2	1:F:256:ILE:CD1	2.39	0.53
1:F:259:ALA:O	1:F:260:LEU:C	2.52	0.53
1:G:255:LYS:HE3	3:G:1299:ADP:O2B	2.08	0.53
1:H:39:MET:CE	1:H:217:LEU:CD2	2.82	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:O	1:H:249:TYR:HD1	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:69:GLY:N	1:J:70:PRO:CD	2.72	0.53
1:J:212:GLU:O	1:J:268:THR:HB	2.09	0.53
1:K:279:ASN:O	1:K:283:LEU:HG	2.09	0.53
1:E:37:ASN:HB2	1:E:219:ASN:CG	2.34	0.53
1:F:235:SER:O	1:F:238:GLN:HB3	2.09	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:32:ILE:HD11	1:E:55:MET:HE1	1.91	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:B:52:VAL:HA	1:B:55:MET:HE2	1.90	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:K:25:PHE:C	1:K:27:GLY:H	2.15	0.53
1:L:89:MET:HE1	1:L:200:LEU:HD11	1.91	0.53
1:E:97:MET:HE3	1:E:158:HIS:HB3	1.90	0.53
1:G:142:THR:HG22	1:G:143:ARG:N	2.16	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:66:HIS:NE2	1:E:109:ASN:HB2	2.24	0.52
1:E:219:ASN:O	1:E:276:ARG:NE	2.42	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:F:97:MET:HE3	1:F:100:VAL:HB	1.91	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:O	1:H:175:LYS:HG2	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:H:199:ASP:CG	1:H:216:LEU:HD21	2.33	0.52
1:I:133:LEU:HD12	1:I:133:LEU:O	2.10	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:D:213:LYS:HZ3	1:D:271:HIS:CE1	2.27	0.52
1:F:261:GLU:O	1:F:265:GLY:N	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:93:ASP:OD2	1:I:96:THR:HG23	2.08	0.52
1:K:131:ALA:N	1:L:123:ALA:O	2.40	0.52
1:B:34:TYR:CE2	1:B:39:MET:HE2	2.44	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:E:30:LEU:HD11	1:E:213:LYS:HG2	1.92	0.52
1:G:39:MET:HG3	1:G:39:MET:O	2.10	0.52
1:H:22:ILE:CD1	1:H:286:PHE:HE2	2.22	0.52
1:H:63:VAL:HG22	1:H:180:PRO:HG2	1.92	0.52
1:H:97:MET:HE1	1:H:195:ASN:CB	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: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: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: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: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:B:218:THR:HG23	1:B:219:ASN:N	2.23	0.51
1:D:3:LEU:HD12	1:F:287:THR:CG2	2.39	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:H:287:THR:HG21	1:L:3:LEU:O	2.10	0.51
1:I:36:GLY:O	1:I:40:GLU:HG2	2.09	0.51
1:I:55:MET:HE3	1:I:285:ILE:CD1	2.33	0.51
1:L:35:GLY:C	1:L:37:ASN:H	2.17	0.51
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:33:LYS:HA	1:E:65:VAL:O	2.11	0.51
1:E:139:LEU:H	1:E:160:GLY:HA2	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:16:SER:O	1:F:17:GLU:C	2.53	0.51
1:F:89:MET:CE	1:F:139:LEU:CD2	2.88	0.51
1:F:219:ASN:C	1:F:219:ASN:ND2	2.65	0.51
1:G:4:SER:OG	1:G:7:ASP:HB2	2.10	0.51
1:G:226:LYS:C	1:G:228:GLY:N	2.61	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:J:19:LEU:HD22	1:K:54:LEU:HD12	1.92	0.51
1:K:34:TYR:CZ	1:K:45:LYS:HE3	2.45	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:F:89:MET:CE	1:F:139:LEU:HD23	2.35	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:L:276:ARG:O	1:L:277:VAL:C	2.52	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: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: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:79:LEU:O	1:J:79:LEU:HG	2.10	0.51
1:J:232:THR:HG23	1:J:294:LEU:HB3	1.93	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:G:75:LEU:C	1:G:79:LEU:HD12	2.36	0.51
1:J:37:ASN:OD1	1:J:37:ASN:N	2.43	0.51
1:J:66:HIS:O	1:J:184:PRO:CD	2.58	0.51
1:K:32:ILE:HG12	1:K:215:MET:HE3	1.93	0.51
1:B:22:ILE:HG22	1:B:26:VAL:HG23	1.93	0.51
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:81:ILE:CG2	1:I:82:GLU:H	2.24	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: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: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:I:10:GLN:O	1:I:14:VAL:HG23	2.11	0.51
1:J:38:ALA:C	1:J:40:GLU:N	2.67	0.51
1:L:22:ILE:CD1	1:L:58:VAL:HG11	2.41	0.51
1:B:30:LEU:CD2	1:B:55:MET:SD	2.99	0.50
1:B:212:GLU:OE1	1:B:212:GLU:HA	2.09	0.50
1:E:93:ASP:OD1	1:E:96:THR:OG1	2.29	0.50
1:E:170:LEU:HD13	1:E:209:LEU:HD11	1.92	0.50
1:G:25:PHE:HB2	1:G:60:ILE:HD13	1.93	0.50
1:H:8:ALA:C	1:L:279:ASN:ND2	2.70	0.50
1:I:79:LEU:HD13	1:J:78:ARG:CG	2.38	0.50
1:J:18:ALA:C	1:J:20:PRO:HD2	2.35	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:K:274:ASP:C	1:K:276:ARG:H	2.19	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:O	1:F:24:ARG:C	2.54	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:B:50:ARG:HB2	1:B:119:HIS:HD2	1.77	0.50
1:E:55:MET:SD	1:E:281:VAL:HG11	2.51	0.50
1:E:251:GLY:O	1:E:254:PRO:HD2	2.11	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:H:270:ALA:C	1:H:271:HIS:HD2	2.20	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:K:257:ARG:O	1:K:261:GLU:HG3	2.12	0.50
1:D:3:LEU:N	1:D:3:LEU:CD2	2.67	0.50
1:E:97:MET:HE1	1:E:195:ASN:CB	2.41	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:212:GLU:C	1:H:213:LYS:HG2	2.36	0.50
1:H:220:ILE:HG21	3:H:1297:ADP:C3'	2.42	0.50
1:I:55:MET:HE3	1:I:281:VAL:HG12	1.94	0.50
1:J:223:LEU:CD1	1:J:248:ILE:HD11	2.38	0.50
1:L:37:ASN:CG	1:L:38:ALA:N	2.69	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:E:35:GLY:C	1:E:39:MET:HG3	2.36	0.50
1:G:190:ASN:HB2	1:G:192:GLU:CD	2.36	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:72:ILE:HG21	1:J:90:ARG:HH22	1.75	0.50
1:J:220:ILE:HD11	3:J:1298:ADP:O3'	2.09	0.50
1:L:8:ALA:O	1:L:9:ALA:C	2.54	0.50
1:A:24:ARG:NH2	1:A:288:ASP:HB2	2.26	0.50
1:A:117:ASN:ND2	1:A:121:GLY:O	2.45	0.50
1:C:32:ILE:HD13	1:C:281:VAL:HG21	1.92	0.50
1:C:90:ARG:NH1	1:I:227:GLN:O	2.45	0.50
1:F:22:ILE:HG21	1:F:58:VAL:CG1	2.42	0.50
1:F:58:VAL:CG1	1:F:58:VAL:O	2.59	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:E:36:GLY:N	1:E:39:MET:HE2	2.26	0.50
1:F:51:ASP:O	1:F:55:MET:HG3	2.12	0.50
1:G:46:ALA:HB1	1:G:119:HIS:HE1	1.76	0.50
1:G:142:THR:CG2	1:G:143:ARG:HD2	2.42	0.50
1:G:172:MET:HG2	1:H:172:MET:HE2	1.92	0.50
1:H:101:GLU:HA	1:H:185:ILE:HD11	1.94	0.50
1:K:75:LEU:CD2	1:L:102:MET:SD	3.00	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:ASP:O	1:A:10:GLN:HB3	2.12	0.50
1:A:39:MET:CE	1:A:39:MET:H	2.25	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: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
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:3:LEU:HD23	1:I:3:LEU:C	2.37	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:39:MET:C	1:H:41:SER:H	2.21	0.49
1:H:220:ILE:CD1	1:H:224:MET:HE3	2.42	0.49
1:H:290:GLY:HA2	1:H:294:LEU:HD13	1.94	0.49
1:K:81:ILE:HG22	1:K:82:GLU:N	2.26	0.49
1:K:213:LYS:HD2	1:K:269:SER:OG	2.12	0.49
1:L:55:MET:O	1:L:60:ILE:N	2.43	0.49
1:A:35:GLY:HA2	1:A:40:GLU:OE1	2.12	0.49
1:A:39:MET:HA	1:A:44:LEU:HD12	1.94	0.49
1:B:15:LEU:HD11	1:C:15:LEU:CD1	2.43	0.49
1:C:58:VAL:O	1:C:58:VAL:CG1	2.60	0.49
1:D:54:LEU:HD13	1:D:282:LEU:HD13	1.94	0.49
1:D:282:LEU:HD11	1:D:286:PHE:CD2	2.48	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:HG22	1:I:154:ILE:O	2.13	0.49
1:J:55:MET:O	1:J:60:ILE:HB	2.12	0.49
1:K:76:LEU:HD21	1:K:99:VAL:HG11	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:216:LEU:HB2	1:K:272:ILE:HG12	1.93	0.49
1:A:235:SER:OG	1:A:238:GLN:NE2	2.45	0.49
1:B:134:ILE:CD1	1:B:201:VAL:HG13	2.42	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: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
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:G:11:VAL:HG22	1:I:15:LEU:HD23	1.93	0.49
1:H:44:LEU:HD23	1:H:275:GLY:O	2.13	0.49
1:I:23:ARG:HG2	1:I:23:ARG:NH1	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:E:79:LEU:O	1:E:80:SER:HB2	2.12	0.49
1:F:199:ASP:C	1:F:258:CYS:SG	2.96	0.49
1:G:102:MET:HE2	1:H:107:GLN:HB2	1.94	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:66:HIS:C	1:G:66:HIS:ND1	2.69	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:O	1:A:58:VAL:HG12	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:H:41:SER:C	1:H:43:GLU:N	2.71	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:L:97:MET:HE3	1:L:100:VAL:HB	1.94	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:188:GLY:HA3	1:D:192:GLU:OE2	2.12	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:I:60:ILE:C	1:I:62:PRO:HD3	2.37	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: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:E:39:MET:HE1	1:E:68:GLY:CA	2.43	0.48
1:H:227:GLN:HG3	1:H:228:GLY:N	2.27	0.48
1:I:42:GLU:O	1:I:45:LYS:HB3	2.13	0.48
1:I:238:GLN:O	1:I:241:GLU:HB2	2.13	0.48
1:K:26:VAL:HG13	1:K:59:GLY:HA3	1.95	0.48
1:K:273:ILE:CD1	1:K:284:GLU:CD	2.85	0.48
1:L:58:VAL:O	1:L:58:VAL:HG12	2.12	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:I:172:MET:HE1	1:J:178:PHE:CE1	2.48	0.48
1:K:5:ARG:CG	1:K:6:ASP:N	2.56	0.48
1:K:213:LYS:HD2	1:K:269:SER:HG	1.78	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:65:VAL:HG21	1:F:202:ALA:HA	1.95	0.48
1:F:291:VAL:O	1:F:291:VAL:HG12	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:J:252:MET:HE1	1:J:255:LYS:HD2	1.91	0.48
1:L:253:LEU:N	1:L:254:PRO:CD	2.76	0.48
1:A:3:LEU:HD13	1:E:286:PHE:O	2.13	0.48
1:E:172:MET:SD	1:F:172:MET:HE3	2.53	0.48
1:E:211:ALA:O	1:E:267:VAL:HG13	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:F:157:GLY:C	1:F:159:VAL:N	2.67	0.48
1:G:9:ALA:HA	1:I:283:LEU:CD2	2.41	0.48
1:G:75:LEU:CG	1:G:79:LEU:HD11	2.36	0.48
1:G:86:ILE:HG22	1:G:87:ASP:N	2.11	0.48
1:H:30:LEU:HD11	1:H:215:MET:HE3	1.94	0.48
1:H:32:ILE:HD13	1:H:281:VAL:HG11	1.95	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:39:MET:HA	1:J:44:LEU:HD12	1.95	0.48
1:K:130:ASP:C	1:K:132:GLU:N	2.70	0.48
1:A:285:ILE:C	1:A:287:THR:N	2.71	0.48
1:A:285:ILE:HG22	1:A:286:PHE:N	2.27	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:75:LEU:HD23	1:H:99:VAL:HG13	1.96	0.48
1:H:229:GLN:HG2	1:H:231:LEU:HD23	1.96	0.48
1:L:30:LEU:HD12	1:L:55:MET:HE1	1.95	0.48
1:A:253:LEU:HB3	1:A:254:PRO:HD3	1.96	0.48
1:C:127:THR:HG22	1:C:183:ALA:HB3	1.95	0.48
1:C:135:ARG:HH21	1:C:164:GLY:HA3	1.79	0.48
1:F:200:LEU:HA	1:F:258:CYS:SG	2.53	0.48
1:F:238:GLN:HA	1:F:241:GLU:CD	2.39	0.48
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:29:THR:HG22	1:I:61:ASN:CB	2.41	0.48
1:I:58:VAL:O	1:I:58:VAL:CG1	2.61	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: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:F:244:ALA:C	1:F:246:GLY:H	2.21	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:7:ASP:HA	1:J:10:GLN:HB2	1.96	0.47
1:J:220:ILE:HD11	3:J:1298:ADP:C2'	2.44	0.47
1:K:172:MET:CE	1:L:173:LEU:HA	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:101:GLU:HA	1:L:185:ILE:HD11	1.95	0.47
1:L:237:GLU:CD	1:L:237:GLU:N	2.72	0.47
1:C:271:HIS:ND1	1:C:284:GLU:OE1	2.47	0.47
1:F:261:GLU:O	1:F:262:ALA:C	2.57	0.47
1:L:38:ALA:C	1:L:40:GLU:N	2.70	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:L:55:MET:HE2	1:L:281:VAL:HG12	1.96	0.47
1:A:263:VAL:HA	1:A:267:VAL:O	2.14	0.47
1:C:33:LYS:C	1:C:33:LYS:HD3	2.39	0.47
1:D:209:LEU:O	1:D:210:LYS:C	2.56	0.47
1:G:214:LEU:HD21	1:G:258:CYS:SG	2.53	0.47
1:I:19:LEU:O	1:I:20:PRO:C	2.56	0.47
1:I:39:MET:HB2	1:I:44:LEU:CD2	2.44	0.47
1:I:66:HIS:O	1:I:184:PRO:CG	2.61	0.47
1:J:19:LEU:N	1:J:20:PRO:CD	2.78	0.47
1:J:73:GLY:O	1:J:77:LYS:HG3	2.14	0.47
1:J:232:THR:CG2	1:J:294:LEU:HB3	2.44	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
1:B:19:LEU:HD13	1:C:54:LEU:HD13	1.96	0.47
1:H:37:ASN:N	1:H:37:ASN:ND2	2.62	0.47
1:I:178:PHE:CE1	1:J:172:MET:CE	2.97	0.47
1:J:113:VAL:HG13	1:J:123:ALA:CB	2.44	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:A:90:ARG:HG2	1:A:91:VAL:O	2.14	0.47
1:A:273:ILE:HD11	1:A:284:GLU:CG	2.45	0.47
1:C:69:GLY:HA2	1:C:71:GLN:HE22	1.79	0.47
1:C:248:ILE:HG21	1:C:256:ILE:HD11	1.97	0.47
1:E:162:VAL:HG11	1:E:204:LYS:HB3	1.97	0.47
1:E:167:VAL:CG1	1:E:171:ASN:HD21	2.26	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:G:252:MET:HE1	1:G:272:ILE:HD12	1.94	0.47
1:H:44:LEU:O	1:H:44:LEU:HG	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:218:THR:CG2	1:H:220:ILE:O	2.63	0.47
1:I:74:ASP:O	1:I:78:ARG:HD3	2.14	0.47
1:I:124:ILE:CD1	1:I:173:LEU:HD22	2.42	0.47
1:J:118:ARG:NH1	1:J:118:ARG:HG3	2.30	0.47
1:J:222:GLY:O	1:J:223:LEU:C	2.58	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:K:229:GLN:HB3	1:K:231:LEU:HD12	1.97	0.47
1:L:19:LEU:O	1:L:22:ILE:N	2.48	0.47
1:A:242:LEU:CD1	1:A:247:THR:HB	2.45	0.47
1:B:34:TYR:CD1	1:B:48:PHE:CE1	3.02	0.47
1:B:237:GLU:O	1:B:241:GLU:HG3	2.15	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:55:MET:HE3	1:G:285:ILE:CD1	2.43	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:24:ARG:HD2	1:K:25:PHE:HE2	1.77	0.47
1:K:192:GLU:O	1:K:194:TYR:CE1	2.68	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:70:PRO:CD	1:F:71:GLN:OE1	2.62	0.47
1:F:77:LYS:HD3	1:F:77:LYS:N	2.29	0.47
1:F:156:ILE:HG22	1:F:159:VAL:HB	1.97	0.47
1:J:25:PHE:CZ	1:J:213:LYS:HE3	2.50	0.47
1:K:60:ILE:C	1:K:62:PRO:HD3	2.37	0.47
1:K:72:ILE:HG12	1:K:103:VAL:CB	2.40	0.47
1:K:124:ILE:HG21	1:K:173:LEU:HD11	1.96	0.47
1:B:212:GLU:O	1:B:268:THR:HB	2.16	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: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:F:139:LEU:CD2	1:F:159:VAL:HG12	2.44	0.46
1:F:139:LEU:HD12	1:F:161:GLU:CG	2.45	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:97:MET:HE1	1:K:195:ASN:N	2.30	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:H:54:LEU:HD21	1:L:15:LEU:HB3	1.97	0.46
1:I:155:ASP:O	1:I:155:ASP:CG	2.58	0.46
1:J:30:LEU:HD12	1:J:60:ILE:HG23	1.95	0.46
1:J:40:GLU:HG3	1:J:40:GLU:H	1.54	0.46
1:L:19:LEU:O	1:L:21:TYR:N	2.48	0.46
1:L:124:ILE:HG22	1:L:126:LEU:HG	1.97	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:I:225:ASP:C	1:I:227:GLN:N	2.69	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:34:TYR:CZ	1:C:39:MET:HB2	2.50	0.46
1:C:162:VAL:HB	1:C:204:LYS:HG3	1.97	0.46
1:D:41:SER:OG	1:D:42:GLU:N	2.48	0.46
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:J:60:ILE:CD1	1:J:285:ILE:HD13	2.45	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:K:123:ALA:O	1:L:131:ALA:N	2.48	0.46
1:L:24:ARG:HG2	1:L:25:PHE:CD1	2.49	0.46
1:L:212:GLU:O	1:L:212:GLU:HG3	2.15	0.46
1:C:69:GLY:HA3	1:C:71:GLN:OE1	2.16	0.46
1:C:97:MET:HE1	1:C:195:ASN:CB	2.29	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:102:MET:HE2	1:J:102:MET:HB2	1.85	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:92:THR:HG22	1:B:97:MET:HB2	1.98	0.46
1:B:261:GLU:HA	1:B:264:GLN:HG2	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:H:94:ALA:O	1:H:97:MET:HB3	2.16	0.46
1:H:253:LEU:O	1:H:254:PRO:C	2.59	0.46
1:I:237:GLU:O	1:I:241:GLU:HG3	2.16	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:H:287:THR:HG22	1:H:288:ASP:N	2.31	0.46
1:J:236:THR:HG23	1:J:240:ASN:HD21	1.81	0.46
1:K:18:ALA:O	1:K:19:LEU:C	2.57	0.46
1:K:31:VAL:HG21	1:K:206:ALA:CA	2.44	0.46
1:K:129:LYS:HZ3	1:K:187:VAL:CG1	2.28	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
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:97:MET:CE	1:F:195:ASN:HB2	2.32	0.46
1:I:255:LYS:HG2	1:I:272:ILE:CD1	2.46	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: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: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:36:GLY:N	1:A:39:MET:HG2	2.30	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:B:54:LEU:CG	1:C:15:LEU:HD23	2.45	0.45
1:B:71:GLN:HG2	1:B:107:GLN:NE2	2.28	0.45
1:B:225:ASP:HB3	1:B:231:LEU:HD11	1.98	0.45
1:D:32:ILE:HD11	1:D:55:MET:HE1	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:252:MET:HE3	1:D:252:MET:HA	1.98	0.45
1:E:136:ALA:CB	1:E:161:GLU:O	2.64	0.45
1:G:19:LEU:HD11	1:I:53:VAL:HG12	1.98	0.45
1:H:196:ILE:CG2	1:H:197:ASN:H	2.28	0.45
1:J:37:ASN:C	1:J:39:MET:N	2.71	0.45
1:J:72:ILE:HD11	1:J:100:VAL:HA	1.98	0.45
1:J:220:ILE:HD11	3:J:1298:ADP:C3'	2.44	0.45
1:A:15:LEU:HB2	1:E:54:LEU:HD21	1.98	0.45
1:B:97:MET:HE1	1:B:195:ASN:H	1.69	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:F:252:MET:HE2	1:F:256:ILE:HD11	1.97	0.45
1:G:54:LEU:O	1:G:55:MET:C	2.58	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:A:31:VAL:HG21	1:A:206:ALA:HB2	1.98	0.45
1:A:234:LEU:CD2	1:A:239:VAL:CG2	2.91	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:39:MET:HE3	1:G:39:MET:CA	2.28	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:G:252:MET:CE	1:G:256:ILE:HG13	2.46	0.45
1:J:23:ARG:NH2	1:K:53:VAL:HG12	2.31	0.45
1:J:92:THR:CG2	1:J:93:ASP:N	2.78	0.45
1:A:29:THR:HA	1:A:61:ASN:O	2.16	0.45
1:A:294:LEU:HG	1:A:294:LEU: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: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:HD12	1:I:19:LEU:HA	1.60	0.45
1:I:224:MET:HE3	1:I:228:GLY:C	2.42	0.45
1:J:28:LYS:HA	1:J:28:LYS:HD2	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:B:52:VAL:HA	1:B:55:MET:CE	2.46	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:F:272:ILE:C	1:F:273:ILE:HG13	2.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:234:LEU:HD21	1:H:242:LEU:HD11	1.98	0.45
1:I:85:PHE:CE2	1:I:90:ARG:HB3	2.52	0.45
1:I:195:ASN:ND2	2:I:1300:NLG:H8C1	2.31	0.45
1:K:58:VAL:HG12	1:K:60:ILE:HG13	1.98	0.45
1:K:90:ARG:HG3	1:K:90:ARG:HH11	1.81	0.45
1:B:34:TYR:HD1	1:B:48:PHE:CE1	2.35	0.45
1:D:115:LEU:HD12	1:D:115:LEU:HA	1.75	0.45
1:G:141:VAL:HG11	1:G:156:ILE:CD1	2.46	0.45
1:G:209:LEU:O	1:G:210:LYS:C	2.59	0.45
1:H:48:PHE:O	1:H:52:VAL:HG23	2.17	0.45
1:H:295:ILE:HG23	1:H:296:SER:N	2.31	0.45
1:I:93:ASP:OD1	1:I:96:THR:HG23	2.16	0.45
1:I:232:THR:HG22	1:I:294:LEU:HB3	1.99	0.45
1:J:34:TYR:CG	1:J:35:GLY:N	2.85	0.45
1:K:66:HIS:O	1:K:184:PRO:HD3	2.16	0.45
1:K:109:ASN:HD22	1:K:110:LYS:N	2.12	0.45
1:L:35:GLY:C	1:L:37:ASN:N	2.72	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
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:L:232:THR:O	1:L:233:GLY:C	2.60	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:B:220:ILE:HG12	1:B:224:MET:HE3	1.99	0.45
1:B:267:VAL:O	1:B:268:THR:C	2.60	0.45
1:C:5:ARG:H	1:C:5:ARG:HD2	1.81	0.45
1:C:92:THR:CG2	1:C:97:MET:HE2	2.45	0.45
1:C:271:HIS:ND1	1:C:294:LEU:HD13	2.32	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:8:ALA:C	1:L:279:ASN:HD21	2.25	0.45
1:I:152:GLU:O	1:I:153:ILE:C	2.58	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:58:VAL:O	1:K:58:VAL:CG1	2.65	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:125:GLY:O	1:E:126:LEU:HD23	2.16	0.45
1:G:167:VAL:O	1:G:167:VAL:HG23	2.17	0.45
1:G:220:ILE:HG13	1:G:221:ALA:N	2.32	0.45
1:I:33:LYS:C	1:I:33:LYS:HD3	2.41	0.45
1:J:124:ILE:O	1:J:124:ILE:HG22	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:4:SER:O	1:A:7:ASP:CB	2.64	0.44
1:A:21:TYR:HD2	1:A:24:ARG:HE	1.65	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:J:74:ASP:C	1:J:74:ASP:OD1	2.60	0.44
1:K:226:LYS:O	1:K:226:LYS:HG3	2.16	0.44
1:L:75:LEU:HD12	1:L:75:LEU:HA	1.69	0.44
1:L:107:GLN:HG2	1:L:108:VAL:N	2.30	0.44
1:L:235:SER:OG	1:L:238:GLN:HG3	2.17	0.44
1:A:30:LEU:HD12	1:A:55:MET:HE3	2.00	0.44
1:B:37:ASN:HB2	1:B:219:ASN:ND2	2.32	0.44
1:C:134:ILE:O	1:C:134:ILE:HG22	2.16	0.44
1:C:225:ASP:O	1:C:227:GLN:N	2.50	0.44
1:D:89:MET:HE2	1:D:159:VAL:HG11	1.97	0.44
1:E:155:ASP:C	1:E:157:GLY:N	2.74	0.44
1:G:85:PHE:O	1:G:86:ILE:O	2.36	0.44
1:G:118:ARG:HH11	1:G:118:ARG:CB	2.29	0.44
1:G:224:MET:HE3	1:G:228:GLY:C	2.42	0.44
1:H:86:ILE:HG22	1:H:87:ASP:HB3	1.99	0.44
1:I:167:VAL:HG11	1:I:208:ALA:O	2.16	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:A:39:MET:H	1:A:39:MET:HE3	1.82	0.44
1:B:29:THR:O	1:B:211:ALA:HB1	2.18	0.44
1:B:143:ARG:HD3	1:B:152:GLU:HB2	1.99	0.44
1:C:74:ASP:OD1	1:I:220:ILE:HG13	2.17	0.44
1:D:166:ASN:C	1:D:166:ASN:OD1	2.59	0.44
1:H:3:LEU:HD21	1:L:283:LEU:HD23	1.98	0.44
1:I:225:ASP:C	1:I:227:GLN:H	2.24	0.44
1:J:15:LEU:CD1	1:K:15:LEU:CD1	2.88	0.44
1:L:128:GLY:HA3	1:L:134:ILE:HB	1.98	0.44
1:B:72:ILE:HD11	1:B:104:LEU:CG	2.47	0.44
1:C:46:ALA:O	1:C:47:GLY:C	2.58	0.44
1:G:55:MET:HG2	1:G:285:ILE:CD1	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:75:LEU:O	1:G:79:LEU:HD12	2.16	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:B:66:HIS:C	1:B:66:HIS:ND1	2.75	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:H:47:GLY:O	1:H:51:ASP:CG	2.61	0.44
1:I:253:LEU:N	1:I:254:PRO:CD	2.81	0.44
1:L:22:ILE:HG12	1:L:58:VAL:HG11	1.99	0.44
1:L:97:MET:O	1:L:98:ASP:C	2.60	0.44
1:A:42:GLU:C	1:A:42:GLU:CD	2.86	0.44
1:B:25:PHE:CE1	1:B:285:ILE:HD12	2.52	0.44
1:D:252:MET:O	1:D:252:MET:HG3	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: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:22:ILE:CG1	1:L:58:VAL:HG11	2.48	0.44
1:L:211:ALA:O	1:L:267:VAL:HG13	2.17	0.44
1:A:10:GLN:O	1:A:14:VAL:CG2	2.66	0.44
1:A:35:GLY:O	1:A:36:GLY:C	2.60	0.44
1:C:2:THR:HG22	1:C:3:LEU:N	2.23	0.44
1:C:43:GLU:OE1	1:I:84:HIS:HA	2.18	0.44
1:F:213:LYS:HA	1:F:269:SER:O	2.17	0.44
1:F:219:ASN:ND2	1:F:219:ASN:N	2.63	0.44
1:H:90:ARG:HD3	1:H:96:THR:CG2	2.48	0.44
1:I:239:VAL:HG21	1:I:256:ILE:HG21	2.00	0.44
1:I:256:ILE:HD12	1:I:295:ILE:CD1	2.43	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:4:SER:O	1:A:5:ARG:C	2.60	0.44
1:A:23:ARG:NH1	1:A:23:ARG:CG	2.78	0.44
1:A:114:ASN:O	1:A:117:ASN:HB2	2.18	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:C:287:THR:C	1:C:289:SER:N	2.74	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:125:GLY:O	1:F:126:LEU:HD23	2.18	0.44
1:G:79:LEU:O	1:G:80:SER:CB	2.60	0.44
1:J:60:ILE:HD11	1:J:285:ILE:HD13	2.00	0.44
1:J:66:HIS:O	1:J:184:PRO:HD3	2.18	0.44
1:J:220:ILE:CD1	3:J:1298:ADP:H2'	2.47	0.44
1:L:220:ILE:HD13	3:L:1300:ADP:N3	2.33	0.44
1:L:255:LYS:NZ	3:L:1300:ADP:O1B	2.34	0.44
1:A:33:LYS:HA	1:A:65:VAL:O	2.18	0.44
1:B:229:GLN:NE2	1:B:229:GLN:HA	2.31	0.44
1:B:252:MET:HE3	1:B:255:LYS:HD2	1.99	0.44
1:C:21:TYR:HD2	1:C:24:ARG:NH1	2.15	0.44
1:C:54:LEU:O	1:C:55:MET:C	2.61	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:I:167:VAL:HG13	1:I:208:ALA:HB1	2.00	0.44
1:K:75:LEU:HD12	1:K:75:LEU:HA	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:G:252:MET:HE3	1:G:256:ILE:HG13	2.00	0.43
1:H:120:GLY:HA3	1:L:23:ARG:HD2	2.00	0.43
1:I:4:SER:O	1:I:5:ARG:C	2.61	0.43
1:I:244:ALA:C	1:I:246:GLY:H	2.25	0.43
1:J:225:ASP:OD1	1:J:225:ASP:O	2.36	0.43
1:K:33:LYS:HB2	1:K:202:ALA:CB	2.48	0.43
1:K:72:ILE:HD11	1:K:104:LEU:CG	2.34	0.43
1:A:170:LEU:HD23	1:A:170:LEU:HA	1.86	0.43
1:B:14:VAL:HG13	1:B:15:LEU:N	2.32	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:42:GLU:O	1:G:43:GLU:C	2.61	0.43
1:G:155:ASP:C	1:G:157:GLY:H	2.25	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:34:TYR:OH	1:C:39:MET:HB2	2.19	0.43
1:C:249:TYR:O	3:C:1300:ADP:H8	2.00	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:K:174:VAL:C	1:K:176:GLY:N	2.73	0.43
1:L:271:HIS:NE2	1:L:284:GLU:OE2	2.47	0.43
1:A:14:VAL:HG11	1:E:11:VAL:HG22	2.00	0.43
1:B:199:ASP:C	1:B:258:CYS:SG	3.01	0.43
1:C:15:LEU:O	1:C:19:LEU:N	2.51	0.43
1:D:75:LEU:HD12	1:D:75:LEU:HA	1.83	0.43
1:F:11:VAL:O	1:F:15:LEU:CG	2.56	0.43
1:F:113:VAL:HG12	1:F:114:ASN:N	2.32	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:5:ARG:HB2	1:J:5:ARG:NH1	2.33	0.43
1:J:51:ASP:O	1:J:54:LEU:HB3	2.19	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:30:LEU:HD21	1:A:213:LYS:HG3	2.00	0.43
1:A:141:VAL:HG21	1:A:156:ILE:HG13	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:89:MET:HE3	1:F:156:ILE:CG2	2.42	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:16:SER:HB3	1:E:50:ARG:CZ	2.49	0.43
1:A:115:LEU:O	1:A:116:ILE:C	2.60	0.43
1:A:223:LEU:H	1:A:293:THR:HG1	1.62	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:F:89:MET:HB3	2:F:1300:NLG:H8C2	2.00	0.43
1:H:139:LEU:HB3	1:H:159:VAL:O	2.19	0.43
1:I:93:ASP:OD2	1:I:93:ASP:C	2.62	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:B:289:SER:C	1:B:291:VAL:H	2.27	0.43
1:C:255:LYS:O	1:C:258:CYS:HB2	2.18	0.43
1:C:287:THR:C	1:C:289:SER:H	2.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:60:ILE:O	1:E:62:PRO:HD3	2.19	0.43
1:E:231:LEU:HD12	1:E:234:LEU:HD11	2.01	0.43
1:F:13:LYS:CG	1:F:14:VAL:N	2.82	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: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:J:188:GLY:CA	1:J:192:GLU:OE2	2.65	0.43
1:K:274:ASP:C	1:K:276:ARG:N	2.74	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:H	1:A:43:GLU:HG3	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:188:GLY:C	1:F:190:ASN:H	2.27	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:52:VAL:O	1:H:55:MET:HB2	2.19	0.43
1:H:145:THR:O	1:H:147:GLU:N	2.46	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:HD23	1:C:242:LEU:HA	1.90	0.43
1:F:77:LYS:HD3	1:F:77:LYS:H	1.84	0.43
1:G:141:VAL:HG12	1:G:142:THR:H	1.82	0.43
1:H:85:PHE:C	1:H:86:ILE:HG13	2.37	0.43
1:H:156:ILE:O	1:H:156:ILE:HG22	2.18	0.43
1:I:213:LYS:HG3	1:I:269:SER:HG	1.82	0.43
1:J:101:GLU:HA	1:J:185:ILE:CD1	2.48	0.43
1:K:32:ILE:HD11	1:K:55:MET:HE1	2.01	0.43
1:L:139:LEU:HD12	1:L:140:THR:H	1.82	0.43
1:C:215:MET:SD	1:C:281:VAL:CG2	3.04	0.43
1:E:76:LEU:HD23	1:E:83:SER:HB3	2.00	0.43
1:E:167:VAL:CG1	1:E:171:ASN:ND2	2.75	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:176:GLY:HA3	1:L:172:MET:HE1	2.01	0.43
1:L:22:ILE:HG21	1:L:58:VAL:CG1	2.49	0.43
1:L:223:LEU:CD1	1:L:256:ILE:HD13	2.45	0.43
1:A:38:ALA:HB3	1:A:219:ASN:OD1	2.19	0.42
1:B:8:ALA:O	1:B:9:ALA:C	2.61	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:H:255:LYS:HZ3	3:H:1297:ADP:PB	2.42	0.42
1:I:39:MET:HA	1:I:44:LEU:HD22	2.00	0.42
1:I:86:ILE:HD13	1:I:154:ILE:CD1	2.49	0.42
1:J:252:MET:SD	3:J:1298:ADP:C2	3.12	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:B:282:LEU:CD2	1:C:8:ALA:HB1	2.49	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:F:72:ILE:O	1:F:73:GLY:C	2.62	0.42
1:G:252:MET:CE	1:G:255:LYS:HD2	2.48	0.42
1:G:283:LEU:HD21	1:I:8:ALA:CB	2.48	0.42
1:H:28:LYS:HD3	1:H:28:LYS:N	2.34	0.42
1:H:232:THR:HG23	1:H:294:LEU:O	2.19	0.42
1:I:39:MET:HE2	1:I:39:MET:HB3	1.97	0.42
1:I:133:LEU:HD12	1:I:133:LEU:C	2.43	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:K:103:VAL:C	1:K:107:GLN:HG2	2.44	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:97:MET:HE1	1:A:195:ASN:N	2.33	0.42
1:A:218:THR:CG2	1:A:255:LYS:HE3	2.45	0.42
1:A:242:LEU:HD13	1:A:242:LEU:HA	1.85	0.42
1:B:137:LYS:H	1:B:163:THR:HG23	1.83	0.42
1:G:36:GLY:O	1:G:39:MET:HB3	2.17	0.42
1:G:101:GLU:OE1	1:G:129:LYS:HE3	2.19	0.42
1:G:150:LYS:O	1:G:151:PRO:C	2.62	0.42
1:G:256:ILE:O	1:G:257:ARG:C	2.63	0.42
1:L:51:ASP:OD1	1:L:282:LEU:HD12	2.19	0.42
1:L:154:ILE:HG23	1:L:154:ILE:O	2.18	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:E:60:ILE:C	1:E:62:PRO:HD3	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:29:THR:HG21	1:A:209:LEU:HD13	2.01	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:B:50:ARG:HH21	1:B:279:ASN:HD21	1.67	0.42
1:B:109:ASN:HD21	1:B:125:GLY:HA3	1.84	0.42
1:D:35:GLY:C	1:D:37:ASN:N	2.72	0.42
1:D:58:VAL:O	1:D:58:VAL:CG1	2.66	0.42
1:D:297:ASN:HB3	1:D:298:ARG:H	1.71	0.42
1:H:34:TYR:CG	1:H:35:GLY:N	2.85	0.42
1:J:225:ASP:OD2	1:J:229:GLN:CB	2.63	0.42
1:K:220:ILE:O	1:K:221:ALA:C	2.61	0.42
1:L:270:ALA:HB3	1:L:295:ILE:HB	2.01	0.42
1:B:115:LEU:HD12	1:B:115:LEU:HA	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:H:206:ALA:HB3	1:H:214:LEU:HD22	2.01	0.42
1:J:37:ASN:O	1:J:38:ALA:C	2.62	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
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: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:90:ARG:HG3	1:K:90:ARG:NH1	2.35	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:277:VAL:CG1	1:K:278:PRO:HD2	2.49	0.42
1:L:22:ILE:HD11	1:L:286:PHE:CZ	2.55	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:L:263:VAL:CG1	1:L:297:ASN:HB2	2.50	0.42
1:D:243:ILE:C	1:D:243:ILE:CD1	2.89	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:E:285:ILE:C	1:E:287:THR:H	2.27	0.42
1:F:29:THR:HG21	1:F:209:LEU:HD13	2.01	0.42
1:G:34:TYR:OH	1:G:45:LYS:HG3	2.20	0.42
1:G:199:ASP:OD1	1:G:255:LYS:HG3	2.19	0.42
1:H:41:SER:O	1:H:42:GLU:C	2.61	0.42
1:H:220:ILE:HG21	3:H:1297:ADP:H3'	2.01	0.42
1:I:3:LEU:HG	1:I:7:ASP:HB3	2.01	0.42
1:I:30:LEU:HD13	1:I:215:MET:HE2	2.01	0.42
1:I:76:LEU:C	1:I:78:ARG:N	2.78	0.42
1:I:260:LEU:O	1:I:264:GLN:HB2	2.20	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:F:138:LYS:HE3	1:F:157:GLY:CA	2.32	0.42
1:F:251:GLY:HA3	3:F:1299:ADP:O2A	2.19	0.42
1:F:259:ALA:O	1:F:262:ALA:HB3	2.20	0.42
1:G:56:LYS:HE2	1:G:177:ASP:HA	2.01	0.42
1:G:115:LEU:HD12	1:G:115:LEU:HA	1.79	0.42
1:I:99:VAL:HG12	1:I:100:VAL:N	2.34	0.42
1:J:67:GLY:O	1:J:68:GLY:C	2.62	0.42
1:K:15:LEU:HA	1:K:15:LEU:HD23	1.77	0.42
1:K:217:LEU:HD22	1:K:275:GLY:HA2	2.02	0.42
1:K:271:HIS:NE2	1:K:294:LEU:HD12	2.34	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
1:F:133:LEU:O	1:F:165:VAL:HA	2.19	0.41
1:F:157:GLY:O	1:F:158:HIS:C	2.62	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:K:37:ASN:O	1:K:39:MET:N	2.53	0.41
1:A:77:LYS:HB2	1:A:77:LYS:HE2	1.80	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:SER:O	1:A:80:SER:OG	2.30	0.41
1:B:170:LEU:HD23	1:B:170:LEU:HA	1.85	0.41
1:K:271:HIS:CD2	1:K:271:HIS:N	2.87	0.41
1:L:19:LEU:C	1:L:21:TYR:N	2.77	0.41
1:L:30:LEU:HD12	1:L:55:MET:SD	2.60	0.41
1:L:232:THR:HG23	1:L:294:LEU:N	2.28	0.41
1:B:19:LEU:N	1:B:20:PRO:CD	2.83	0.41
1:C:16:SER:C	1:C:18:ALA:N	2.78	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:I:57:ALA:C	1:I:59:GLY:H	2.29	0.41
1:I:127:THR:C	1:I:129:LYS:N	2.78	0.41
1:I:215:MET:HE1	1:I:281:VAL:CG1	2.51	0.41
1:J:273:ILE:CG2	1:J:274:ASP:N	2.83	0.41
1:K:21:TYR:CD1	1:K:21:TYR:N	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:B:195:ASN:C	2:B:1302:NLG:H8C1	2.46	0.41
1:D:2:THR:HG23	1:D:2:THR:O	2.20	0.41
1:F:209:LEU:O	1:F:210:LYS:C	2.63	0.41
1:F:219:ASN:HD21	3:F:1299:ADP:H5'1	1.85	0.41
1:F:252:MET:HE1	1:F:272:ILE:HD13	2.02	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:I:93:ASP:O	1:I:94:ALA:C	2.64	0.41
1:K:24:ARG:HH12	1:K:288:ASP:CA	2.33	0.41
1:K:124:ILE:HG22	1:K:126:LEU:CG	2.50	0.41
1:K:193:SER:C	1:K:194:TYR:CD1	2.99	0.41
1:L:85:PHE:C	1:L:86:ILE:HG13	2.45	0.41
1:A:33:LYS:CE	1:A:199:ASP:OD2	2.64	0.41
1:B:30:LEU:HD21	1:B:215:MET:HE2	2.02	0.41
1:B:34:TYR:HD2	1:B:39:MET:HE3	1.84	0.41
1:B:51:ASP:O	1:B:55:MET:HG3	2.20	0.41
1:B:144:GLN:CD	1:B:149:THR:CG2	2.94	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:3:LEU:CD2	1:L:283:LEU:HD23	2.51	0.41
1:H:24:ARG:HG3	1:H:25:PHE:CE2	2.55	0.41
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:L:34:TYR:HA	1:L:217:LEU:HD12	2.02	0.41
1:L:250:GLY:C	1:L:252:MET:H	2.27	0.41
1:A:172:MET:HE1	1:B:173:LEU:HD23	2.03	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:O	1:G:156:ILE:CG2	2.68	0.41
1:G:187:VAL:HA	1:G:192:GLU:O	2.20	0.41
1:J:31:VAL:HG11	1:J:202:ALA:O	2.21	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:K:25:PHE:CD1	1:K:285:ILE:HB	2.55	0.41
1:K:195:ASN:ND2	2:K:1298:NLG:O	2.49	0.41
1:A:31:VAL:HG21	1:A:206:ALA:HA	2.02	0.41
1:A:139:LEU:N	1:A:160:GLY:HA2	2.34	0.41
1:B:252:MET:CE	1:B:255:LYS:HB3	2.47	0.41
1:C:60:ILE:O	1:C:62:PRO:HD3	2.21	0.41
1:C:298:ARG:O	1:C:299:LYS:HB2	2.20	0.41
1:H:19:LEU:CD2	1:L:53:VAL:CG1	2.98	0.41
1:L:22:ILE:CG2	1:L:58:VAL:CG1	2.99	0.41
1:C:223:LEU:C	1:C:223:LEU:CD1	2.86	0.41
1:G:273:ILE:HG23	1:G:274:ASP:N	2.35	0.41
1:H:5:ARG:CG	1:H:6:ASP:N	2.83	0.41
1:I:55:MET:CE	1:I:215:MET:HE1	2.40	0.41
1:I:127:THR:C	1:I:129:LYS:H	2.28	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:37:ASN:CG	1:L:38:ALA:H	2.28	0.41
1:L:76:LEU:CD1	1:L:90:ARG:NH2	2.83	0.41
1:L:156:ILE:HG22	1:L:159:VAL:CG2	2.40	0.41
1:A:30:LEU:CD1	1:A:55:MET:CE	2.96	0.41
1:B:14:VAL:CG2	1:C:3:LEU:HD13	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:141:VAL:CG1	1:B:142:THR:H	2.34	0.41
1:B:220:ILE:O	1:B:221:ALA:C	2.64	0.41
1:B:225:ASP:OD2	1:B:225:ASP:C	2.63	0.41
1:C:16:SER:O	1:C:19:LEU:HB2	2.20	0.41
1:C:258:CYS:O	1:C:259:ALA:C	2.64	0.41
1:D:96:THR:O	1:D:100:VAL:HG23	2.21	0.41
1:D:107:GLN:O	1:D:111:ASP:HB3	2.20	0.41
1:E:289:SER:HB2	1:E:291:VAL:CG1	2.50	0.41
1:F:219:ASN:HD22	1:F:219:ASN:N	2.19	0.41
1:G:25:PHE:O	1:G:26:VAL:C	2.61	0.41
1:H:55:MET:HB3	1:H:55:MET:HE2	1.85	0.41
1:H:144:GLN:O	1:H:146:PRO:HD3	2.20	0.41
1:J:11:VAL:O	1:J:12:ALA:C	2.62	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:25:PHE:C	1:K:27:GLY:N	2.79	0.41
1:K:37:ASN:O	1:K:38:ALA:C	2.62	0.41
1:K:72:ILE:CG1	1:K:103:VAL:CG1	2.97	0.41
1:K:271:HIS:CE1	1:K:284:GLU:HG3	2.55	0.41
1:K:274:ASP:HB3	1:K:277:VAL:HG23	2.03	0.41
1:L:19:LEU:HB3	1:L:20:PRO:CD	2.44	0.41
1:A:41:SER:O	1:A:45:LYS:HG3	2.21	0.41
1:D:40:GLU:C	1:D:41:SER:O	2.64	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:I:225:ASP:HB3	1:I:229:GLN:H	1.85	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:B:220:ILE:CG1	1:B:224:MET:HE3	2.51	0.40
1:C:28:LYS:CG	1:C:29:THR:N	2.65	0.40
1:C:29:THR:HG21	1:C:209:LEU:HD13	2.03	0.40
1:C:232:THR:O	1:C:233:GLY:C	2.63	0.40
1:D:54:LEU:HD11	1:F:15:LEU:CD1	2.47	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:72:ILE:CD1	1:E:104:LEU:HG	2.49	0.40
1:H:12:ALA:CB	1:L:50:ARG:HH21	2.28	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:HD23	1:K:76:LEU:HA	1.90	0.40
1:L:55:MET:SD	1:L:60:ILE:HG21	2.61	0.40
1:A:215:MET:HE1	1:A:285:ILE:HD11	2.02	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:252:MET:HE2	1:G:256:ILE:CG1	2.52	0.40
1:G:287:THR:HG22	1:G:288:ASP:H	1.85	0.40
1:H:27:GLY:C	1:H:28:LYS:HD3	2.47	0.40
1:H:262:ALA:O	1:H:263:VAL:C	2.63	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:J:123:ALA:C	1:J:124:ILE:HD12	2.45	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
1:A:55:MET:O	1:A:60:ILE:HG13	2.21	0.40
1:C:70:PRO:HD2	1:C:71:GLN:NE2	2.36	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: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:188:GLY:C	1:F:190:ASN:N	2.77	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:2:THR:O	1:J:3:LEU:HB2	2.21	0.40
1:J:30:LEU:HD23	1:J:213:LYS:HB2	1.96	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:31:VAL:HG21	1:A:206:ALA:CB	2.52	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:C:5:ARG:CG	1:C:5:ARG:NH1	2.84	0.40
1:C:55:MET:CE	1:C:285:ILE:HD13	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:169:LEU:HD12	1:E:172:MET:HE2	2.03	0.40
1:E:218:THR:CB	1:E:255:LYS:HE2	2.51	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:I:66:HIS:O	1:I:184:PRO:CD	2.69	0.40
1:L:54:LEU:HD11	1:L:286:PHE:HZ	1.87	0.40
1:A:11:VAL:HG22	1:E:15:LEU:HD23	2.03	0.40
1:B:248:ILE:HG23	1:B:252:MET:CG	2.52	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:E:42:GLU:O	1:E:43:GLU:C	2.64	0.40
1:E:142:THR:C	1:E:154:ILE:CB	2.95	0.40
1:G:29:THR:HG22	1:G:211:ALA:HB2	2.04	0.40
1:H:72:ILE:O	1:H:76:LEU:HG	2.21	0.40
1:H:145:THR:CG2	1:H:147:GLU:OE2	2.69	0.40
1:I:56:LYS:HD2	1:I:56:LYS:HA	1.85	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:OE1	1:I:284:GLU:HA	2.21	0.40
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:J:128:GLY:HA3	1:J:185:ILE:O	2.22	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: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%)	<b>7</b> <b>20</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	293/300 (98%)	268 (92%)	23 (8%)	2 (1%)	18	40
1	C	297/300 (99%)	272 (92%)	20 (7%)	5 (2%)	7	20
1	D	291/300 (97%)	272 (94%)	14 (5%)	5 (2%)	7	20
1	E	284/300 (95%)	250 (88%)	28 (10%)	6 (2%)	5	16
1	F	288/300 (96%)	242 (84%)	38 (13%)	8 (3%)	4	11
1	G	296/300 (99%)	254 (86%)	33 (11%)	9 (3%)	3	9
1	H	294/300 (98%)	243 (83%)	36 (12%)	15 (5%)	1	3
1	I	285/300 (95%)	254 (89%)	28 (10%)	3 (1%)	11	29
1	J	276/300 (92%)	221 (80%)	40 (14%)	15 (5%)	1	3
1	K	268/300 (89%)	221 (82%)	36 (13%)	11 (4%)	2	5
1	L	290/300 (97%)	243 (84%)	37 (13%)	10 (3%)	3	7
All	All	3450/3600 (96%)	2989 (87%)	367 (11%)	94 (3%)	4	11

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

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
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
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

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Mol	Chain	Res	Type
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
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 [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	231/239 (97%)	185 (80%)	46 (20%)	<b>1</b> <b>3</b>

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	233/239 (98%)	203 (87%)	30 (13%)	4	13
1	C	237/239 (99%)	213 (90%)	24 (10%)	7	20
1	D	233/239 (98%)	201 (86%)	32 (14%)	3	11
1	E	225/239 (94%)	181 (80%)	44 (20%)	1	3
1	F	226/239 (95%)	193 (85%)	33 (15%)	3	9
1	G	235/239 (98%)	189 (80%)	46 (20%)	1	3
1	H	234/239 (98%)	196 (84%)	38 (16%)	2	7
1	I	225/239 (94%)	189 (84%)	36 (16%)	2	8
1	J	210/239 (88%)	188 (90%)	22 (10%)	6	19
1	K	188/239 (79%)	162 (86%)	26 (14%)	3	10
1	L	232/239 (97%)	183 (79%)	49 (21%)	1	2
All	All	2709/2868 (94%)	2283 (84%)	426 (16%)	2	8

All (426) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	5	ARG
1	A	6	ASP
1	A	7	ASP
1	A	11	VAL
1	A	14	VAL
1	A	23	ARG
1	A	24	ARG
1	A	39	MET
1	A	55	MET
1	A	58	VAL
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	138	LYS
1	A	142	THR
1	A	153	ILE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	187	VAL
1	A	192	GLU
1	A	220	ILE
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	245	ASP
1	A	247	THR
1	A	253	LEU
1	A	256	ILE
1	A	264	GLN
1	A	278	PRO
1	A	281	VAL
1	A	286	PHE
1	A	287	THR
1	A	289	SER
1	A	291	VAL
1	A	294	LEU
1	A	299	LYS
1	A	300	ARG
1	B	16	SER
1	B	40	GLU
1	B	41	SER
1	B	45	LYS
1	B	54	LEU
1	B	58	VAL
1	B	71	GLN
1	B	76	LEU
1	B	83	SER
1	B	85	PHE
1	B	115	LEU
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	154	ILE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
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	282	LEU
1	B	291	VAL
1	C	2	THR
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	58	VAL
1	C	71	GLN
1	C	134	ILE
1	C	138	LYS
1	C	145	THR
1	C	167	VAL
1	C	187	VAL
1	C	217	LEU
1	C	223	LEU
1	C	232	THR
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	D	3	LEU
1	D	4	SER
1	D	5	ARG
1	D	29	THR
1	D	43	GLU
1	D	58	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	D	70	PRO
1	D	83	SER
1	D	107	GLN
1	D	111	ASP
1	D	113	VAL
1	D	126	LEU
1	D	143	ARG
1	D	145	THR
1	D	151	PRO
1	D	153	ILE
1	D	156	ILE
1	D	167	VAL
1	D	192	GLU
1	D	214	LEU
1	D	215	MET
1	D	217	LEU
1	D	219	ASN
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
1	E	30	LEU
1	E	52	VAL
1	E	54	LEU
1	E	70	PRO
1	E	71	GLN
1	E	72	ILE
1	E	74	ASP
1	E	77	LYS
1	E	92	THR
1	E	93	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	E	101	GLU
1	E	111	ASP
1	E	113	VAL
1	E	142	THR
1	E	153	ILE
1	E	156	ILE
1	E	161	GLU
1	E	163	THR
1	E	175	LYS
1	E	189	SER
1	E	193	SER
1	E	213	LYS
1	E	219	ASN
1	E	220	ILE
1	E	227	GLN
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	267	VAL
1	E	269	SER
1	E	281	VAL
1	E	287	THR
1	E	291	VAL
1	E	298	ARG
1	F	11	VAL
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
1	F	113	VAL
1	F	134	ILE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	F	142	THR
1	F	143	ARG
1	F	153	ILE
1	F	154	ILE
1	F	167	VAL
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	256	ILE
1	F	258	CYS
1	F	281	VAL
1	F	288	ASP
1	F	294	LEU
1	G	11	VAL
1	G	29	THR
1	G	30	LEU
1	G	41	SER
1	G	42	GLU
1	G	43	GLU
1	G	52	VAL
1	G	58	VAL
1	G	60	ILE
1	G	71	GLN
1	G	72	ILE
1	G	82	GLU
1	G	83	SER
1	G	85	PHE
1	G	86	ILE
1	G	90	ARG
1	G	102	MET
1	G	103	VAL
1	G	115	LEU
1	G	118	ARG
1	G	126	LEU
1	G	142	THR
1	G	143	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	G	144	GLN
1	G	146	PRO
1	G	147	GLU
1	G	151	PRO
1	G	152	GLU
1	G	153	ILE
1	G	161	GLU
1	G	167	VAL
1	G	189	SER
1	G	192	GLU
1	G	199	ASP
1	G	212	GLU
1	G	214	LEU
1	G	220	ILE
1	G	257	ARG
1	G	258	CYS
1	G	260	LEU
1	G	263	VAL
1	G	269	SER
1	G	272	ILE
1	G	273	ILE
1	G	287	THR
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	56	LYS
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

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	H	174	VAL
1	H	175	LYS
1	H	187	VAL
1	H	212	GLU
1	H	214	LEU
1	H	215	MET
1	H	220	ILE
1	H	230	VAL
1	H	231	LEU
1	H	235	SER
1	H	243	ILE
1	H	249	TYR
1	H	258	CYS
1	H	267	VAL
1	H	268	THR
1	H	271	HIS
1	H	281	VAL
1	H	288	ASP
1	H	289	SER
1	I	3	LEU
1	I	5	ARG
1	I	7	ASP
1	I	10	GLN
1	I	19	LEU
1	I	26	VAL
1	I	71	GLN
1	I	78	ARG
1	I	80	SER
1	I	81	ILE
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	104	LEU
1	I	111	ASP
1	I	118	ARG
1	I	129	LYS
1	I	139	LEU
1	I	153	ILE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	I	154	ILE
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	237	GLU
1	I	243	ILE
1	I	255	LYS
1	I	263	VAL
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
1	J	72	ILE
1	J	80	SER
1	J	86	ILE
1	J	92	THR
1	J	101	GLU
1	J	118	ARG
1	J	192	GLU
1	J	195	ASN
1	J	201	VAL
1	J	219	ASN
1	J	226	LYS
1	J	229	GLN
1	J	234	LEU
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	26	VAL
1	K	41	SER
1	K	58	VAL
1	K	80	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	K	82	GLU
1	K	83	SER
1	K	97	MET
1	K	99	VAL
1	K	100	VAL
1	K	109	ASN
1	K	124	ILE
1	K	126	LEU
1	K	129	LYS
1	K	172	MET
1	K	199	ASP
1	K	200	LEU
1	K	230	VAL
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	6	ASP
1	L	17	GLU
1	L	22	ILE
1	L	26	VAL
1	L	33	LYS
1	L	39	MET
1	L	41	SER
1	L	55	MET
1	L	72	ILE
1	L	78	ARG
1	L	81	ILE
1	L	85	PHE
1	L	87	ASP
1	L	99	VAL
1	L	108	VAL
1	L	112	ILE
1	L	113	VAL
1	L	124	ILE
1	L	129	LYS
1	L	134	ILE
1	L	143	ARG
1	L	156	ILE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	L	161	GLU
1	L	172	MET
1	L	192	GLU
1	L	193	SER
1	L	200	LEU
1	L	201	VAL
1	L	205	VAL
1	L	213	LYS
1	L	220	ILE
1	L	227	GLN
1	L	229	GLN
1	L	240	ASN
1	L	241	GLU
1	L	243	ILE
1	L	245	ASP
1	L	252	MET
1	L	256	ILE
1	L	258	CYS
1	L	276	ARG
1	L	277	VAL
1	L	278	PRO
1	L	287	THR
1	L	291	VAL
1	L	296	SER
1	L	297	ASN
1	L	299	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (77) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	10	GLN
1	A	37	ASN
1	A	84	HIS
1	A	117	ASN
1	A	238	GLN
1	A	240	ASN
1	B	71	GLN
1	B	107	GLN
1	B	109	ASN
1	B	119	HIS
1	B	195	ASN
1	B	219	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	229	GLN
1	B	238	GLN
1	B	240	ASN
1	B	264	GLN
1	B	279	ASN
1	C	264	GLN
1	D	107	GLN
1	D	119	HIS
1	D	219	ASN
1	D	229	GLN
1	E	84	HIS
1	E	117	ASN
1	E	171	ASN
1	E	190	ASN
1	E	195	ASN
1	E	238	GLN
1	F	37	ASN
1	F	171	ASN
1	F	219	ASN
1	F	240	ASN
1	G	107	GLN
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	190	ASN
1	H	195	ASN
1	H	197	ASN
1	H	219	ASN
1	H	264	GLN
1	H	271	HIS
1	I	107	GLN
1	I	109	ASN
1	I	117	ASN
1	I	227	GLN
1	I	271	HIS
1	J	195	ASN
1	J	219	ASN

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Mol	Chain	Res	Type
1	J	229	GLN
1	J	240	ASN
1	J	264	GLN
1	J	297	ASN
1	K	66	HIS
1	K	84	HIS
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	144	GLN
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 oligosaccharides 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	J	1298	-	28,29,29	2.23	9 (32%)	43,45,45	1.72	11 (25%)
2	NLG	F	1300	-	12,12,12	4.19	6 (50%)	15,15,15	4.33	9 (60%)
3	ADP	H	1297	4	28,29,29	1.90	7 (25%)	43,45,45	1.60	9 (20%)
3	ADP	G	1299	4	28,29,29	1.69	6 (21%)	43,45,45	1.54	9 (20%)
2	NLG	E	1301	-	12,12,12	4.29	6 (50%)	15,15,15	4.29	7 (46%)
3	ADP	C	1300	4	28,29,29	1.78	5 (17%)	43,45,45	1.64	10 (23%)
2	NLG	A	1302	-	12,12,12	4.15	7 (58%)	15,15,15	4.32	8 (53%)
3	ADP	D	1300	4	28,29,29	1.52	3 (10%)	43,45,45	1.44	8 (18%)
2	NLG	B	1302	-	12,12,12	4.29	6 (50%)	15,15,15	4.28	7 (46%)
3	ADP	I	1298	4	28,29,29	1.50	3 (10%)	43,45,45	1.39	7 (16%)
2	NLG	G	1301	-	12,12,12	4.20	6 (50%)	15,15,15	4.37	10 (66%)
3	ADP	E	1299	4	28,29,29	1.76	5 (17%)	43,45,45	1.56	9 (20%)
2	NLG	L	1302	-	12,12,12	4.25	7 (58%)	15,15,15	4.27	8 (53%)
3	ADP	L	1300	4	28,29,29	1.70	5 (17%)	43,45,45	1.55	9 (20%)
2	NLG	K	1298	-	12,12,12	4.09	6 (50%)	15,15,15	4.47	9 (60%)
3	ADP	B	1300	4	28,29,29	1.83	7 (25%)	43,45,45	1.52	8 (18%)
2	NLG	H	1299	-	12,12,12	4.37	7 (58%)	15,15,15	4.32	9 (60%)
2	NLG	D	1302	-	12,12,12	4.20	5 (41%)	15,15,15	4.29	8 (53%)
2	NLG	I	1300	-	12,12,12	4.17	6 (50%)	15,15,15	4.33	9 (60%)
3	ADP	F	1299	-	28,29,29	1.71	6 (21%)	43,45,45	1.50	7 (16%)

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	J	1298	-	-	2/16/32/32	0/3/3/3
2	NLG	F	1300	-	-	0/13/13/13	-
3	ADP	H	1297	4	-	6/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	G	1299	4	-	3/16/32/32	0/3/3/3
2	NLG	E	1301	-	-	0/13/13/13	-
3	ADP	C	1300	4	-	2/16/32/32	0/3/3/3
2	NLG	A	1302	-	-	0/13/13/13	-
3	ADP	D	1300	4	-	4/16/32/32	0/3/3/3
2	NLG	B	1302	-	-	0/13/13/13	-
3	ADP	I	1298	4	-	3/16/32/32	0/3/3/3
2	NLG	G	1301	-	-	1/13/13/13	-
3	ADP	E	1299	4	-	4/16/32/32	0/3/3/3
2	NLG	L	1302	-	-	1/13/13/13	-
3	ADP	L	1300	4	-	6/16/32/32	0/3/3/3
2	NLG	K	1298	-	-	1/13/13/13	-
3	ADP	B	1300	4	-	2/16/32/32	0/3/3/3
2	NLG	H	1299	-	-	1/13/13/13	-
2	NLG	D	1302	-	-	1/13/13/13	-
2	NLG	I	1300	-	-	1/13/13/13	-
3	ADP	F	1299	-	-	4/16/32/32	0/3/3/3

All (118) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	1299	NLG	C8-C7	-10.25	1.29	1.50
2	G	1301	NLG	C8-C7	-10.04	1.29	1.50
2	B	1302	NLG	C8-C7	-9.65	1.30	1.50
2	D	1302	NLG	C8-C7	-9.63	1.30	1.50
2	K	1298	NLG	C8-C7	-9.59	1.30	1.50
2	E	1301	NLG	C8-C7	-9.47	1.30	1.50
2	F	1300	NLG	C8-C7	-9.40	1.31	1.50
2	A	1302	NLG	C8-C7	-9.38	1.31	1.50
2	I	1300	NLG	C8-C7	-9.36	1.31	1.50
2	L	1302	NLG	C8-C7	-9.30	1.31	1.50
2	L	1302	NLG	CA-C	-7.11	1.34	1.52
2	E	1301	NLG	CA-C	-6.82	1.35	1.52
2	B	1302	NLG	CA-C	-6.81	1.35	1.52
2	D	1302	NLG	C7-N2	-6.81	1.12	1.34
2	E	1301	NLG	C7-N2	-6.78	1.12	1.34
2	F	1300	NLG	CA-C	-6.78	1.35	1.52
2	H	1299	NLG	C7-N2	-6.78	1.12	1.34
2	I	1300	NLG	CA-C	-6.71	1.35	1.52
2	A	1302	NLG	C7-N2	-6.67	1.12	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	1299	NLG	CA-C	-6.49	1.36	1.52
2	D	1302	NLG	CA-C	-6.47	1.36	1.52
2	F	1300	NLG	C7-N2	-6.43	1.13	1.34
2	L	1302	NLG	C7-N2	-6.33	1.14	1.34
2	B	1302	NLG	C7-N2	-6.30	1.14	1.34
2	G	1301	NLG	C7-N2	-6.28	1.14	1.34
2	I	1300	NLG	C7-N2	-6.23	1.14	1.34
2	K	1298	NLG	CA-C	-6.15	1.37	1.52
2	G	1301	NLG	CA-C	-6.10	1.37	1.52
2	A	1302	NLG	CA-C	-6.01	1.37	1.52
2	K	1298	NLG	C7-N2	-5.97	1.15	1.34
3	E	1299	ADP	C4-N3	5.55	1.44	1.34
3	J	1298	ADP	C4-N3	5.35	1.44	1.34
3	H	1297	ADP	PA-O3A	5.34	1.65	1.59
3	B	1300	ADP	C4-N3	5.19	1.44	1.34
3	D	1300	ADP	C4-N3	5.11	1.44	1.34
3	F	1299	ADP	C4-N3	5.10	1.43	1.34
3	L	1300	ADP	C4-N3	5.10	1.43	1.34
3	C	1300	ADP	C4-N3	5.07	1.43	1.34
3	H	1297	ADP	C4-N3	4.95	1.43	1.34
3	I	1298	ADP	C4-N3	4.65	1.43	1.34
3	G	1299	ADP	C4-N3	4.48	1.42	1.34
2	B	1302	NLG	CA-N2	4.33	1.54	1.45
3	J	1298	ADP	C3'-C4'	-4.28	1.42	1.53
3	F	1299	ADP	C2-N1	4.18	1.41	1.33
3	E	1299	ADP	C2-N1	4.16	1.41	1.33
3	B	1300	ADP	C2-N1	4.10	1.41	1.33
3	L	1300	ADP	C2-N1	4.04	1.41	1.33
3	C	1300	ADP	C2-N1	4.03	1.41	1.33
2	I	1300	NLG	CA-N2	4.02	1.54	1.45
2	L	1302	NLG	CA-N2	3.99	1.54	1.45
3	H	1297	ADP	C2-N1	3.94	1.40	1.33
2	A	1302	NLG	CA-N2	3.87	1.53	1.45
3	D	1300	ADP	C2-N1	3.86	1.40	1.33
3	J	1298	ADP	O3'-C3'	3.85	1.52	1.43
3	G	1299	ADP	C2-N1	3.83	1.40	1.33
3	J	1298	ADP	PA-O3A	3.73	1.63	1.59
3	I	1298	ADP	C2-N1	3.73	1.40	1.33
2	F	1300	NLG	CA-N2	3.70	1.53	1.45
3	J	1298	ADP	C2-N1	3.67	1.40	1.33
2	E	1301	NLG	CA-N2	3.61	1.53	1.45
2	H	1299	NLG	CA-N2	3.52	1.53	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1300	ADP	PA-O3A	3.45	1.63	1.59
2	K	1298	NLG	CA-N2	3.30	1.52	1.45
2	D	1302	NLG	CA-N2	3.24	1.52	1.45
3	J	1298	ADP	O4'-C1'	3.23	1.49	1.42
2	B	1302	NLG	OXT-C	3.10	1.40	1.30
2	G	1301	NLG	CA-N2	2.94	1.52	1.45
3	C	1300	ADP	PA-O3A	2.94	1.62	1.59
2	K	1298	NLG	OXT-C	2.87	1.39	1.30
2	D	1302	NLG	OXT-C	2.84	1.39	1.30
2	E	1301	NLG	OXT-C	2.84	1.39	1.30
2	L	1302	NLG	OXT-C	2.79	1.39	1.30
2	I	1300	NLG	OXT-C	2.78	1.39	1.30
2	G	1301	NLG	OXT-C	2.75	1.39	1.30
3	G	1299	ADP	PA-O3A	2.74	1.62	1.59
2	A	1302	NLG	OXT-C	2.70	1.39	1.30
2	H	1299	NLG	OXT-C	2.66	1.39	1.30
3	G	1299	ADP	C5-N7	-2.65	1.34	1.39
2	E	1301	NLG	CB-CG	2.64	1.60	1.52
2	F	1300	NLG	OXT-C	2.60	1.38	1.30
3	F	1299	ADP	PA-O3A	2.51	1.62	1.59
3	L	1300	ADP	PA-O2A	-2.48	1.43	1.55
3	L	1300	ADP	C5-N7	-2.44	1.34	1.39
2	A	1302	NLG	CB-CG	2.43	1.60	1.52
3	E	1299	ADP	O3'-C3'	2.43	1.49	1.43
3	J	1298	ADP	C2'-C3'	2.42	1.59	1.53
3	E	1299	ADP	C6-N1	2.39	1.42	1.35
3	B	1300	ADP	O3'-C3'	2.34	1.48	1.43
2	B	1302	NLG	CB-CG	2.34	1.59	1.52
3	B	1300	ADP	C5-N7	-2.31	1.34	1.39
3	F	1299	ADP	C6-N1	2.26	1.42	1.35
2	G	1301	NLG	O-C	2.25	1.28	1.22
3	J	1298	ADP	C6-N1	2.24	1.42	1.35
3	H	1297	ADP	PA-O2A	-2.24	1.45	1.55
2	A	1302	NLG	O-C	2.22	1.28	1.22
3	G	1299	ADP	C6-N1	2.22	1.42	1.35
3	B	1300	ADP	C6-N1	2.21	1.42	1.35
3	H	1297	ADP	C5-N7	-2.20	1.35	1.39
2	L	1302	NLG	O-C	2.20	1.28	1.22
2	H	1299	NLG	O-C	2.19	1.28	1.22
2	L	1302	NLG	CB-CG	2.17	1.59	1.52
3	F	1299	ADP	PA-O2A	-2.14	1.45	1.55
2	H	1299	NLG	CB-CG	2.14	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1300	ADP	C6-N1	2.13	1.41	1.35
3	H	1297	ADP	C6-N1	2.12	1.41	1.35
3	I	1298	ADP	PA-O2A	-2.10	1.45	1.55
3	B	1300	ADP	PA-O2A	-2.08	1.45	1.55
3	F	1299	ADP	C5-N7	-2.08	1.35	1.39
3	E	1299	ADP	PA-O2A	-2.07	1.45	1.55
3	H	1297	ADP	O3'-C3'	2.07	1.48	1.43
3	C	1300	ADP	C6-N1	2.07	1.41	1.35
2	I	1300	NLG	O-C	2.06	1.28	1.22
3	L	1300	ADP	C6-N1	2.05	1.41	1.35
3	C	1300	ADP	O3'-C3'	2.05	1.48	1.43
3	J	1298	ADP	C8-N9	2.04	1.41	1.37
3	G	1299	ADP	PA-O2A	-2.04	1.45	1.55
2	K	1298	NLG	O-C	2.03	1.28	1.22
2	F	1300	NLG	O-C	2.01	1.28	1.22

All (171) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	1298	NLG	OXT-C-O	-10.48	100.31	124.08
2	G	1301	NLG	OXT-C-O	-10.39	100.50	124.08
2	H	1299	NLG	OXT-C-O	-10.34	100.63	124.08
2	F	1300	NLG	OXT-C-O	-10.33	100.65	124.08
2	A	1302	NLG	OXT-C-O	-10.32	100.66	124.08
2	I	1300	NLG	OXT-C-O	-10.23	100.88	124.08
2	D	1302	NLG	OXT-C-O	-10.16	101.03	124.08
2	B	1302	NLG	OXT-C-O	-10.04	101.29	124.08
2	E	1301	NLG	OXT-C-O	-9.96	101.48	124.08
2	L	1302	NLG	OXT-C-O	-9.95	101.50	124.08
2	K	1298	NLG	C8-C7-N2	7.30	128.22	116.12
2	G	1301	NLG	C8-C7-N2	7.09	127.88	116.12
2	B	1302	NLG	CA-N2-C7	6.88	140.87	121.58
2	L	1302	NLG	C8-C7-N2	6.87	127.52	116.12
2	A	1302	NLG	C8-C7-N2	6.83	127.44	116.12
2	I	1300	NLG	C8-C7-N2	6.81	127.42	116.12
2	E	1301	NLG	C8-C7-N2	6.77	127.35	116.12
2	H	1299	NLG	C8-C7-N2	6.66	127.16	116.12
2	D	1302	NLG	C8-C7-N2	6.63	127.12	116.12
2	F	1300	NLG	C8-C7-N2	6.55	126.97	116.12
2	B	1302	NLG	C8-C7-N2	6.54	126.96	116.12
2	F	1300	NLG	CA-N2-C7	6.52	139.86	121.58
2	E	1301	NLG	CA-N2-C7	6.49	139.77	121.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1302	NLG	CA-N2-C7	6.36	139.41	121.58
2	I	1300	NLG	CA-N2-C7	6.29	139.22	121.58
2	L	1302	NLG	CA-N2-C7	6.17	138.87	121.58
2	D	1302	NLG	CA-N2-C7	5.99	138.36	121.58
2	H	1299	NLG	CA-N2-C7	5.90	138.12	121.58
2	K	1298	NLG	CB-CG-CD	-5.60	97.57	112.49
2	E	1301	NLG	O7-C7-N2	-5.35	112.53	121.98
2	D	1302	NLG	O7-C7-N2	-5.32	112.57	121.98
2	A	1302	NLG	O7-C7-N2	-5.30	112.62	121.98
2	K	1298	NLG	O7-C7-N2	-5.26	112.69	121.98
2	G	1301	NLG	O7-C7-N2	-5.23	112.74	121.98
2	L	1302	NLG	O7-C7-N2	-5.22	112.76	121.98
2	I	1300	NLG	O7-C7-N2	-5.15	112.89	121.98
2	H	1299	NLG	OXT-C-CA	5.09	130.75	113.51
2	H	1299	NLG	O7-C7-N2	-5.09	112.98	121.98
2	K	1298	NLG	OXT-C-CA	5.04	130.57	113.51
2	G	1301	NLG	OXT-C-CA	5.03	130.53	113.51
2	D	1302	NLG	OXT-C-CA	4.99	130.41	113.51
2	F	1300	NLG	OXT-C-CA	4.99	130.40	113.51
2	F	1300	NLG	O7-C7-N2	-4.96	113.21	121.98
2	B	1302	NLG	OXT-C-CA	4.96	130.29	113.51
2	I	1300	NLG	OXT-C-CA	4.94	130.21	113.51
2	E	1301	NLG	OXT-C-CA	4.90	130.08	113.51
2	G	1301	NLG	CA-N2-C7	4.90	135.31	121.58
2	L	1302	NLG	OXT-C-CA	4.83	129.85	113.51
2	K	1298	NLG	CA-N2-C7	4.83	135.11	121.58
2	B	1302	NLG	O7-C7-N2	-4.78	113.53	121.98
2	A	1302	NLG	OXT-C-CA	4.69	129.38	113.51
3	J	1298	ADP	O5'-C5'-C4'	4.68	124.93	108.99
2	G	1301	NLG	CB-CG-CD	-4.60	100.22	112.49
3	E	1299	ADP	C4-N9-C1'	4.31	136.72	126.63
3	L	1300	ADP	C4-N9-C1'	4.06	136.12	126.63
3	C	1300	ADP	C4-N9-C1'	3.80	135.52	126.63
3	F	1299	ADP	C4-N9-C1'	3.73	135.35	126.63
3	G	1299	ADP	C4-N9-C1'	3.63	135.12	126.63
3	H	1297	ADP	C4-N9-C1'	3.62	135.10	126.63
3	B	1300	ADP	C4-N9-C1'	3.55	134.94	126.63
3	H	1297	ADP	C4-N9-C8	-3.50	102.07	105.74
2	A	1302	NLG	OE2-CD-CG	-3.47	103.03	114.00
3	C	1300	ADP	N9-C8-N7	3.47	118.86	113.94
2	B	1302	NLG	OE2-CD-CG	-3.47	103.04	114.00
3	C	1300	ADP	C4-N9-C8	-3.46	102.11	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	1299	ADP	C4-N9-C8	-3.41	102.15	105.74
2	F	1300	NLG	OE2-CD-CG	-3.40	103.24	114.00
2	D	1302	NLG	OE1-CD-CG	3.36	133.75	123.09
2	D	1302	NLG	OE2-CD-CG	-3.36	103.40	114.00
2	A	1302	NLG	OE1-CD-CG	3.36	133.73	123.09
2	E	1301	NLG	OE2-CD-CG	-3.34	103.44	114.00
3	J	1298	ADP	C4-N9-C8	-3.33	102.24	105.74
2	F	1300	NLG	OE1-CD-CG	3.33	133.66	123.09
2	H	1299	NLG	OE1-CD-CG	3.32	133.62	123.09
2	E	1301	NLG	OE1-CD-CG	3.32	133.61	123.09
3	H	1297	ADP	N9-C8-N7	3.30	118.62	113.94
3	F	1299	ADP	N9-C8-N7	3.29	118.60	113.94
2	B	1302	NLG	OE1-CD-CG	3.27	133.45	123.09
3	E	1299	ADP	N9-C8-N7	3.26	118.56	113.94
3	L	1300	ADP	N9-C8-N7	3.26	118.56	113.94
3	G	1299	ADP	C4-N9-C8	-3.25	102.32	105.74
3	B	1300	ADP	N9-C8-N7	3.25	118.55	113.94
3	L	1300	ADP	C4-N9-C8	-3.25	102.33	105.74
2	H	1299	NLG	OE2-CD-CG	-3.16	104.03	114.00
3	C	1300	ADP	C5-C6-N6	3.15	131.09	123.29
3	I	1298	ADP	C4-N9-C1'	3.13	133.96	126.63
3	G	1299	ADP	N9-C8-N7	3.13	118.38	113.94
3	B	1300	ADP	C4-N9-C8	-3.13	102.45	105.74
2	I	1300	NLG	OE1-CD-CG	3.11	132.96	123.09
2	I	1300	NLG	CB-CG-CD	-3.11	104.20	112.49
2	I	1300	NLG	OE2-CD-CG	-3.10	104.21	114.00
2	L	1302	NLG	OE1-CD-CG	3.09	132.89	123.09
2	D	1302	NLG	CB-CG-CD	-3.08	104.28	112.49
3	J	1298	ADP	C5-C6-N6	3.08	130.90	123.29
3	J	1298	ADP	N6-C6-N1	-3.08	111.53	118.38
3	D	1300	ADP	C5-C6-N6	3.00	130.71	123.29
2	L	1302	NLG	OE2-CD-CG	-3.00	104.53	114.00
2	G	1301	NLG	OE1-CD-CG	2.99	132.58	123.09
3	E	1299	ADP	C1'-N9-C8	-2.98	120.49	127.09
3	D	1300	ADP	N6-C6-N1	-2.95	111.81	118.38
3	F	1299	ADP	C5-C6-N6	2.93	130.54	123.29
3	I	1298	ADP	C4-N9-C8	-2.92	102.67	105.74
3	H	1297	ADP	C5-C6-N6	2.90	130.47	123.29
2	G	1301	NLG	OE2-CD-CG	-2.89	104.87	114.00
3	I	1298	ADP	C5-C6-N6	2.88	130.41	123.29
3	C	1300	ADP	N6-C6-N1	-2.88	111.97	118.38
3	I	1298	ADP	N6-C6-N1	-2.87	111.98	118.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1300	ADP	C2'-C1'-N9	-2.87	106.17	113.30
3	E	1299	ADP	C4-N9-C8	-2.81	102.79	105.74
3	I	1298	ADP	N9-C8-N7	2.80	117.91	113.94
3	J	1298	ADP	O4'-C4'-C5'	2.78	118.25	109.33
3	J	1298	ADP	C2'-C1'-N9	-2.77	106.41	113.30
2	K	1298	NLG	OE1-CD-CG	2.77	131.87	123.09
3	C	1300	ADP	O5'-C5'-C4'	2.77	118.41	108.99
3	G	1299	ADP	C5-C6-N6	2.76	130.12	123.29
2	L	1302	NLG	CB-CG-CD	-2.76	105.14	112.49
3	B	1300	ADP	C5-C6-N6	2.75	130.10	123.29
3	H	1297	ADP	N6-C6-N1	-2.69	112.38	118.38
3	E	1299	ADP	O3'-C3'-C4'	-2.67	103.40	111.08
3	F	1299	ADP	N6-C6-N1	-2.67	112.43	118.38
3	L	1300	ADP	C5-C6-N6	2.67	129.90	123.29
3	H	1297	ADP	O3'-C3'-C4'	-2.65	103.48	111.08
3	J	1298	ADP	C2'-C3'-C4'	2.64	107.71	102.61
3	J	1298	ADP	C4-N9-C1'	2.64	132.80	126.63
2	K	1298	NLG	OE2-CD-CG	-2.63	105.69	114.00
3	D	1300	ADP	C4-N9-C1'	2.62	132.75	126.63
3	I	1298	ADP	O3'-C3'-C4'	-2.62	103.56	111.08
3	J	1298	ADP	O4'-C4'-C3'	-2.61	99.96	105.15
2	H	1299	NLG	C-CA-N2	-2.61	104.51	110.57
3	J	1298	ADP	N9-C8-N7	2.60	117.62	113.94
3	E	1299	ADP	C5-C6-N6	2.60	129.72	123.29
3	D	1300	ADP	C4-N9-C8	-2.59	103.02	105.74
3	C	1300	ADP	C3'-C2'-C1'	2.57	106.32	101.46
3	J	1298	ADP	O2A-PA-O3A	2.54	114.13	107.27
3	L	1300	ADP	N6-C6-N1	-2.51	112.78	118.38
2	H	1299	NLG	CB-CG-CD	-2.50	105.82	112.49
3	L	1300	ADP	C1'-N9-C8	-2.50	121.54	127.09
3	D	1300	ADP	N9-C8-N7	2.49	117.47	113.94
2	F	1300	NLG	CB-CG-CD	-2.47	105.91	112.49
3	E	1299	ADP	N6-C6-N1	-2.47	112.88	118.38
3	B	1300	ADP	N6-C6-N1	-2.46	112.89	118.38
3	G	1299	ADP	N6-C6-N1	-2.43	112.97	118.38
3	L	1300	ADP	O3'-C3'-C4'	-2.42	104.13	111.08
3	H	1297	ADP	O4'-C4'-C3'	-2.39	100.40	105.15
3	C	1300	ADP	O2A-PA-O3A	2.39	113.72	107.27
2	A	1302	NLG	O-C-CA	2.38	129.95	122.26
3	D	1300	ADP	O3'-C3'-C4'	-2.33	104.38	111.08
2	G	1301	NLG	C-CA-N2	-2.32	105.18	110.57
3	L	1300	ADP	C3'-C2'-C1'	2.32	105.85	101.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	1297	ADP	O2A-PA-O3A	2.28	113.45	107.27
3	B	1300	ADP	C3'-C2'-C1'	2.25	105.71	101.46
3	G	1299	ADP	O4'-C4'-C3'	-2.24	100.70	105.15
3	I	1298	ADP	C3'-C2'-C1'	2.22	105.67	101.46
3	F	1299	ADP	C3'-C2'-C1'	2.22	105.66	101.46
3	D	1300	ADP	C3'-C2'-C1'	2.19	105.61	101.46
3	B	1300	ADP	C4-C5-N7	2.19	113.09	110.58
3	E	1299	ADP	C3'-C2'-C1'	2.17	105.58	101.46
2	K	1298	NLG	O-C-CA	2.13	129.13	122.26
3	C	1300	ADP	C1'-N9-C8	-2.13	122.37	127.09
3	G	1299	ADP	O2A-PA-O3A	2.12	113.01	107.27
3	E	1299	ADP	C4-C5-N7	2.12	113.01	110.58
2	G	1301	NLG	O-C-CA	2.08	128.95	122.26
2	F	1300	NLG	O-C-CA	2.08	128.95	122.26
3	F	1299	ADP	C1'-N9-C8	-2.07	122.49	127.09
3	G	1299	ADP	C1'-N9-C8	-2.06	122.51	127.09
2	I	1300	NLG	O-C-CA	2.06	128.91	122.26
3	B	1300	ADP	C1'-N9-C8	-2.06	122.53	127.09
3	G	1299	ADP	O5'-C5'-C4'	2.05	115.97	108.99
3	L	1300	ADP	C4-C5-N7	2.04	112.92	110.58
3	C	1300	ADP	O3'-C3'-C4'	-2.02	105.28	111.08
3	H	1297	ADP	C1'-N9-C8	-2.01	122.64	127.09

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1300	ADP	PA-O3A-PB-O3B
3	C	1300	ADP	C4'-C5'-O5'-PA
3	J	1298	ADP	PA-O3A-PB-O3B
3	J	1298	ADP	C4'-C5'-O5'-PA
2	H	1299	NLG	CA-CB-CG-CD
2	K	1298	NLG	CA-CB-CG-CD
3	D	1300	ADP	C4'-C5'-O5'-PA
3	E	1299	ADP	C4'-C5'-O5'-PA
3	F	1299	ADP	C4'-C5'-O5'-PA
3	I	1298	ADP	C4'-C5'-O5'-PA
2	D	1302	NLG	CA-CB-CG-CD
3	C	1300	ADP	PA-O3A-PB-O1B
3	F	1299	ADP	C2'-C1'-N9-C4
2	L	1302	NLG	CA-CB-CG-CD
3	B	1300	ADP	C4'-C5'-O5'-PA

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Mol	Chain	Res	Type	Atoms
3	G	1299	ADP	C4'-C5'-O5'-PA
3	H	1297	ADP	C4'-C5'-O5'-PA
3	L	1300	ADP	C4'-C5'-O5'-PA
2	I	1300	NLG	CA-CB-CG-CD
3	F	1299	ADP	C2'-C1'-N9-C8
3	D	1300	ADP	PA-O3A-PB-O1B
2	G	1301	NLG	CA-CB-CG-CD
3	D	1300	ADP	PA-O3A-PB-O2B
3	D	1300	ADP	PA-O3A-PB-O3B
3	H	1297	ADP	PA-O3A-PB-O2B
3	H	1297	ADP	PA-O3A-PB-O3B
3	L	1300	ADP	PA-O3A-PB-O2B
3	L	1300	ADP	PA-O3A-PB-O3B
3	E	1299	ADP	C2'-C1'-N9-C8
3	L	1300	ADP	C2'-C1'-N9-C8
3	E	1299	ADP	C2'-C1'-N9-C4
3	E	1299	ADP	O4'-C1'-N9-C8
3	G	1299	ADP	O4'-C1'-N9-C8
3	H	1297	ADP	O4'-C1'-N9-C8
3	L	1300	ADP	O4'-C1'-N9-C8
3	F	1299	ADP	O4'-C1'-N9-C8
3	I	1298	ADP	O4'-C1'-N9-C8
3	G	1299	ADP	C2'-C1'-N9-C8
3	H	1297	ADP	C2'-C1'-N9-C8
3	I	1298	ADP	C2'-C1'-N9-C8
3	L	1300	ADP	C2'-C1'-N9-C4
3	H	1297	ADP	PA-O3A-PB-O1B

There are no ring outliers.

16 monomers are involved in 55 short contacts:

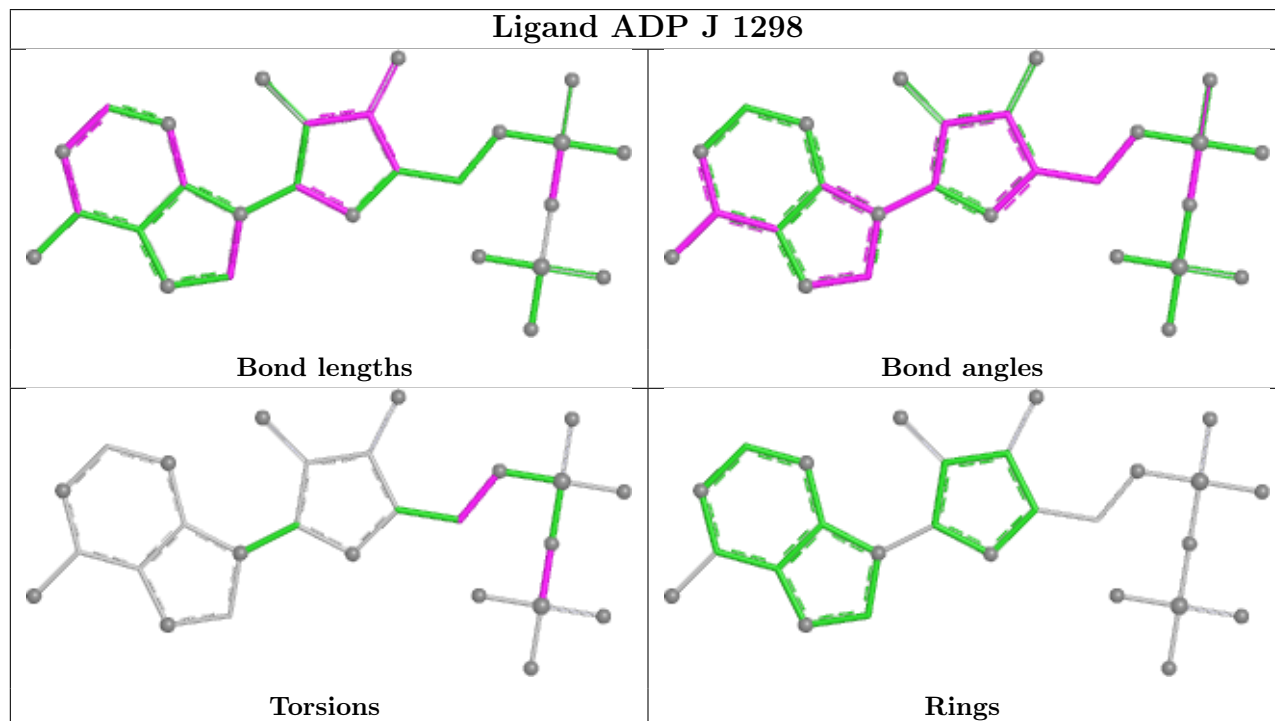
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	J	1298	ADP	13	0
2	F	1300	NLG	3	0
3	H	1297	ADP	5	0
3	G	1299	ADP	1	0
3	C	1300	ADP	2	0
2	B	1302	NLG	1	0
2	G	1301	NLG	4	0
3	E	1299	ADP	3	0
2	L	1302	NLG	3	0
3	L	1300	ADP	4	0

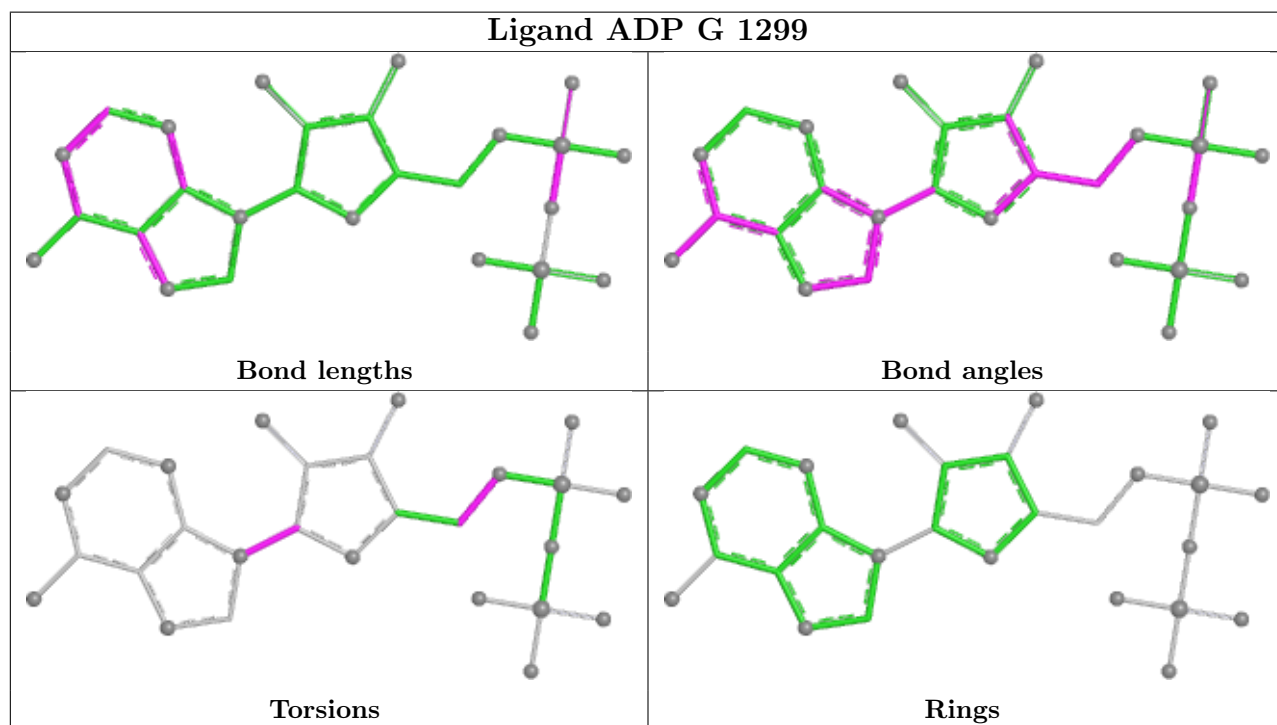
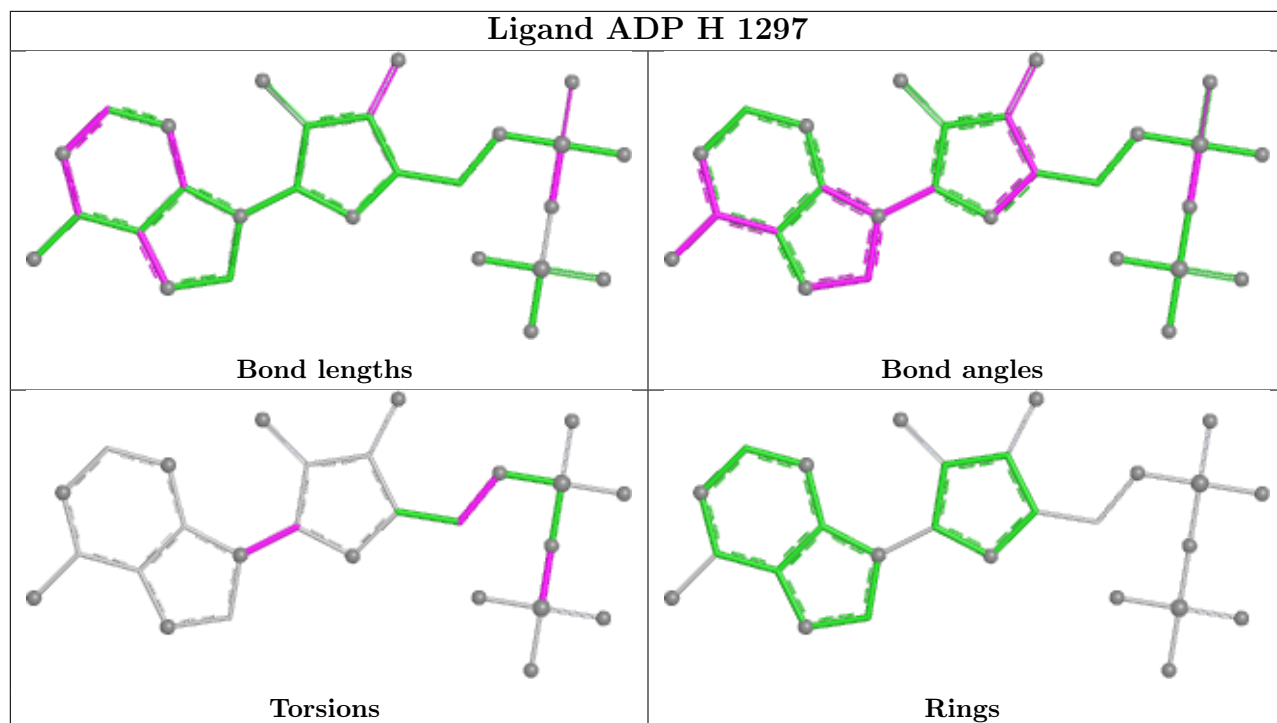
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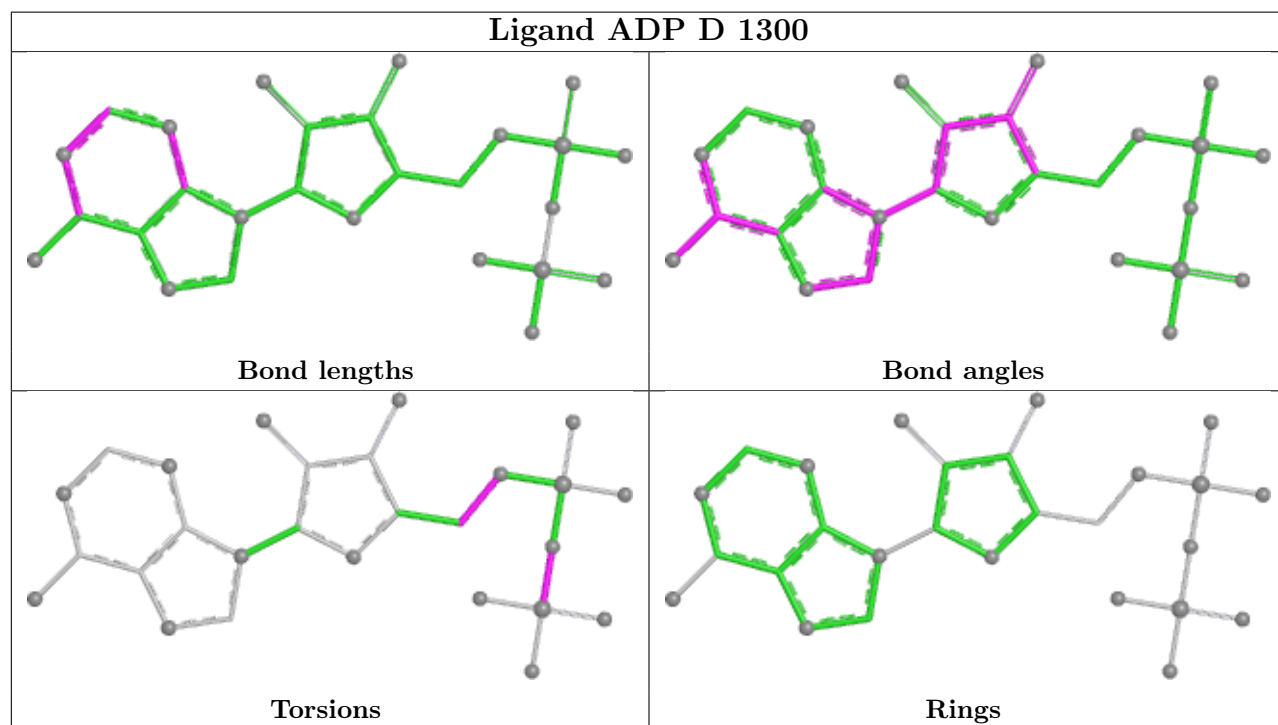
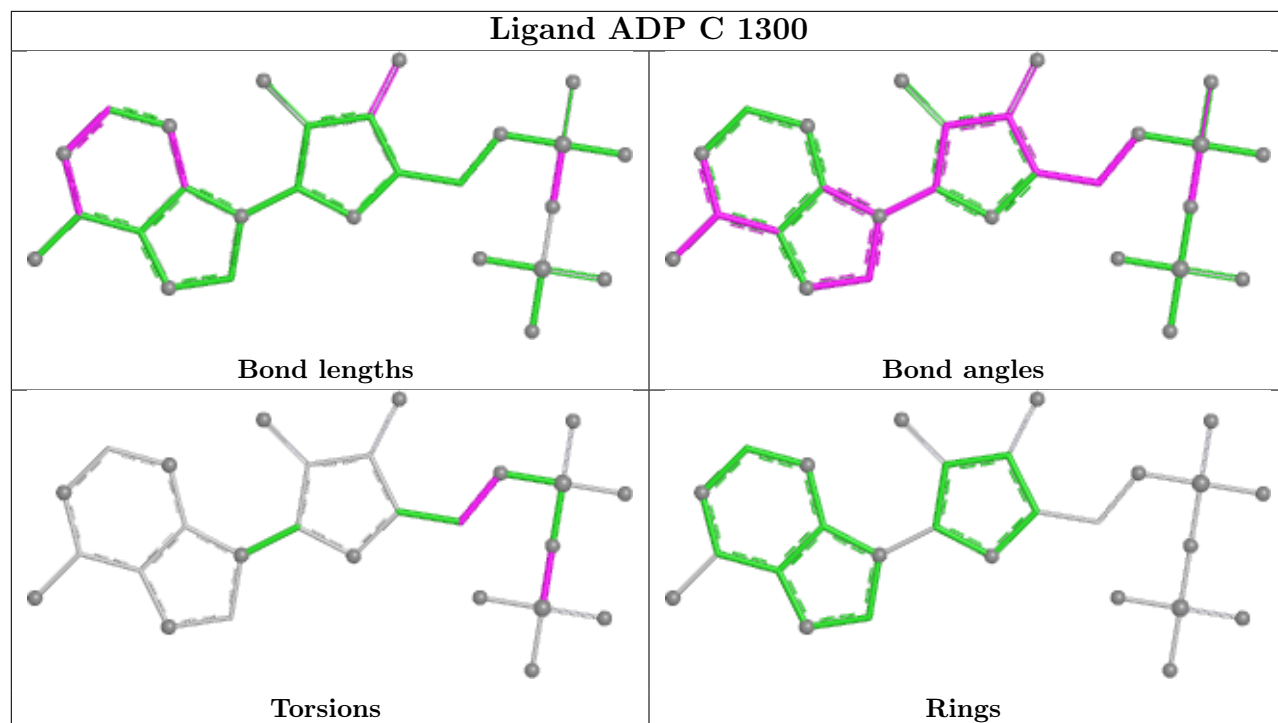
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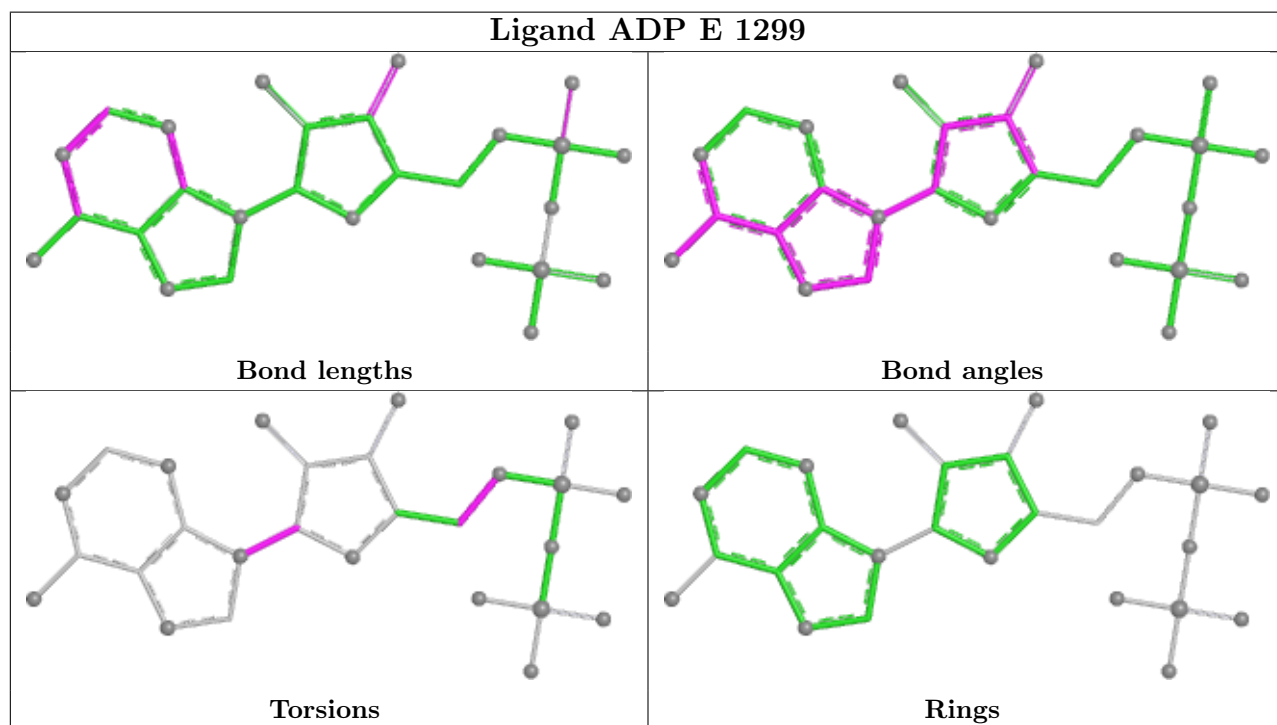
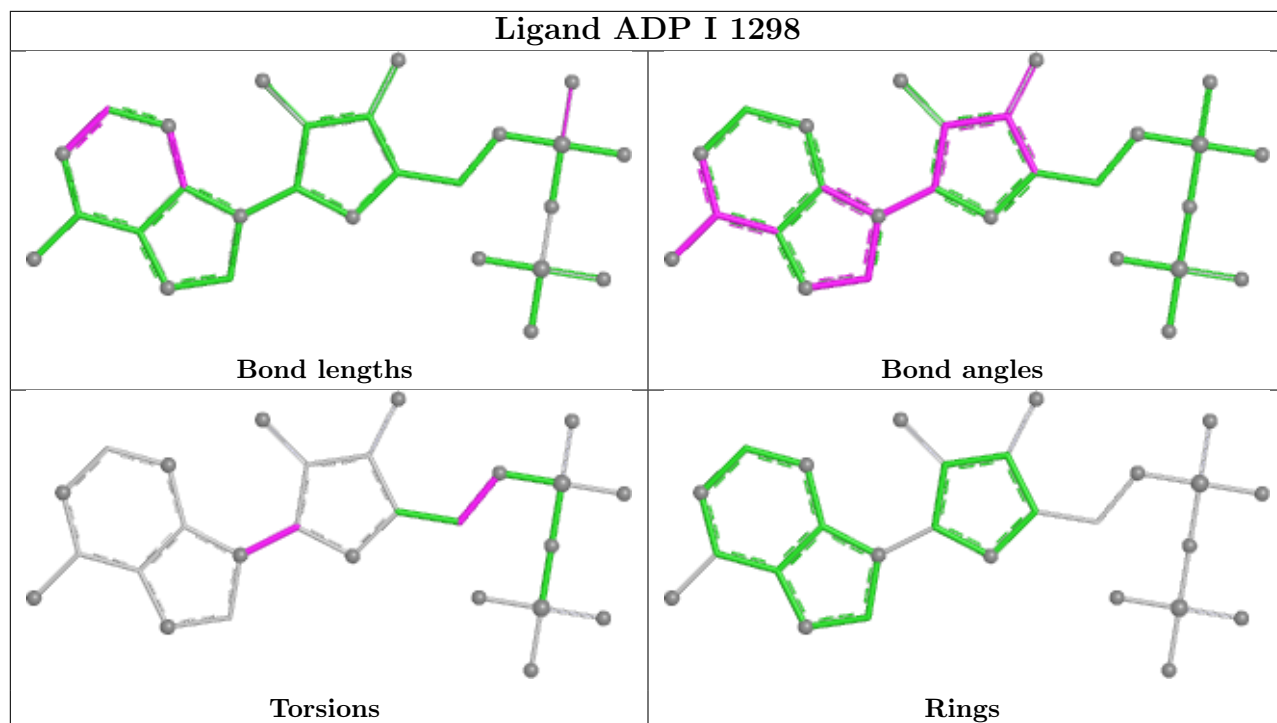
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	K	1298	NLG	4	0
3	B	1300	ADP	2	0
2	H	1299	NLG	6	0
2	D	1302	NLG	1	0
2	I	1300	NLG	1	0
3	F	1299	ADP	2	0

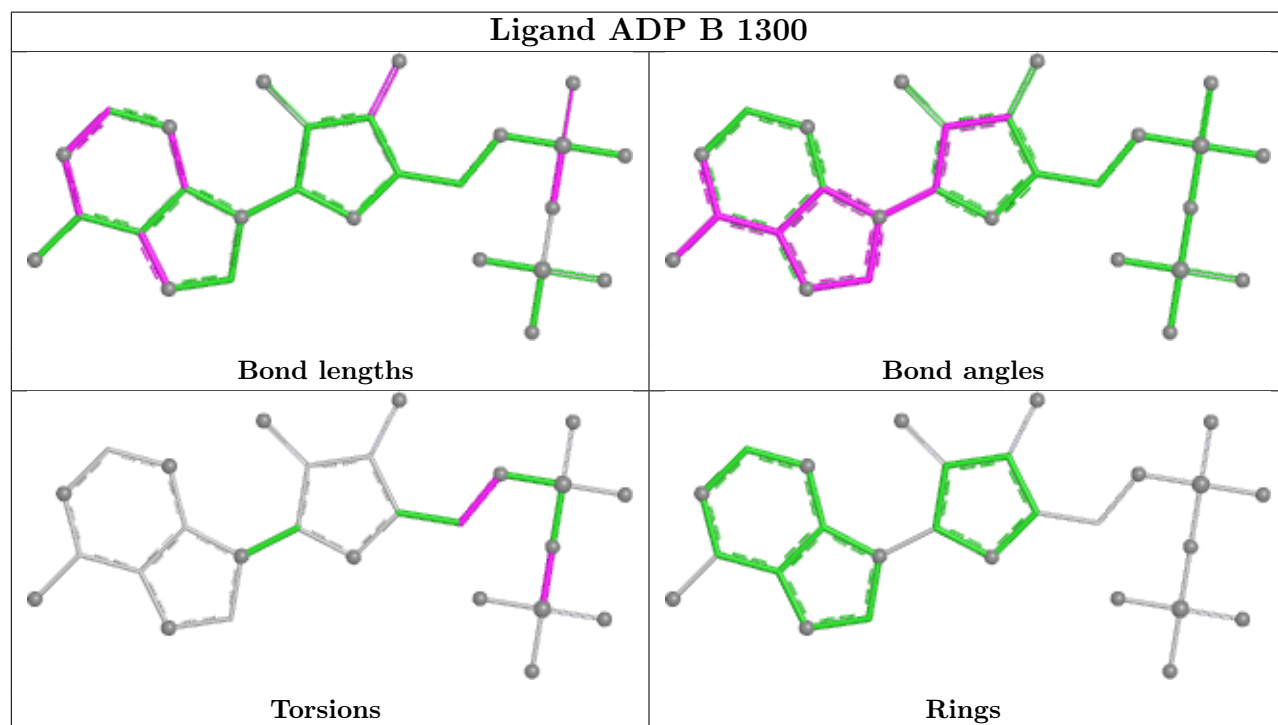
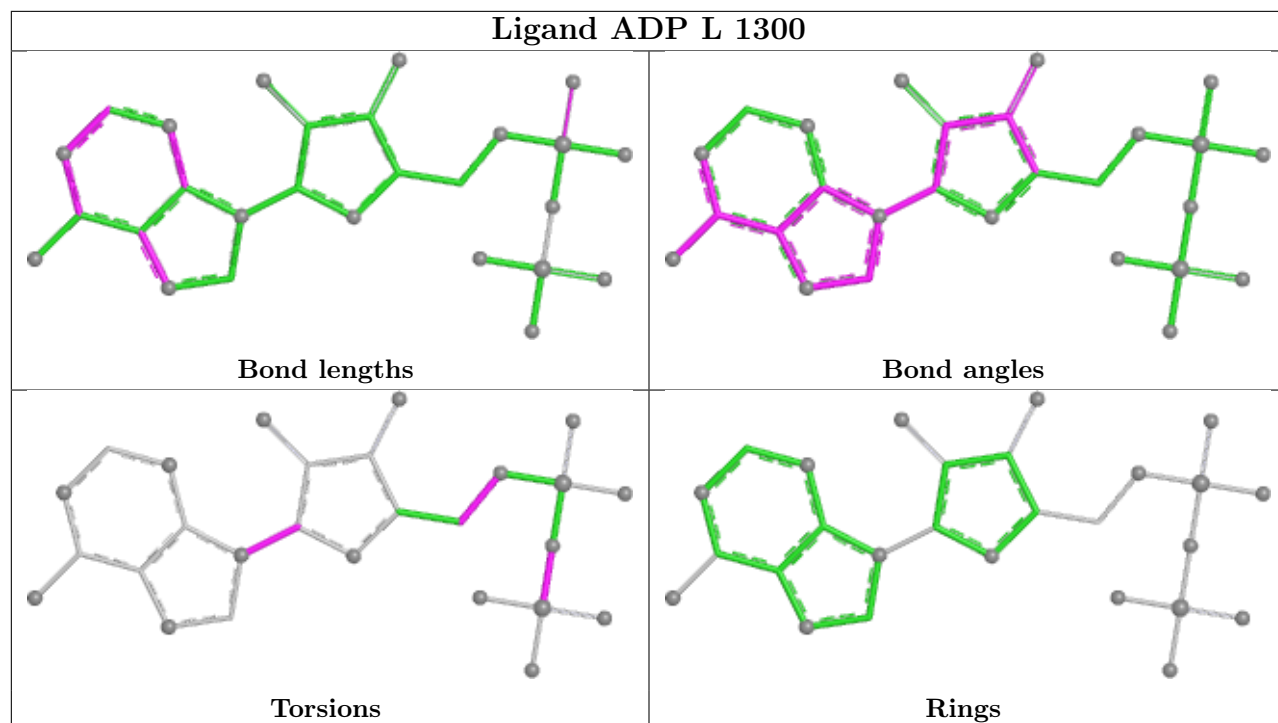
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

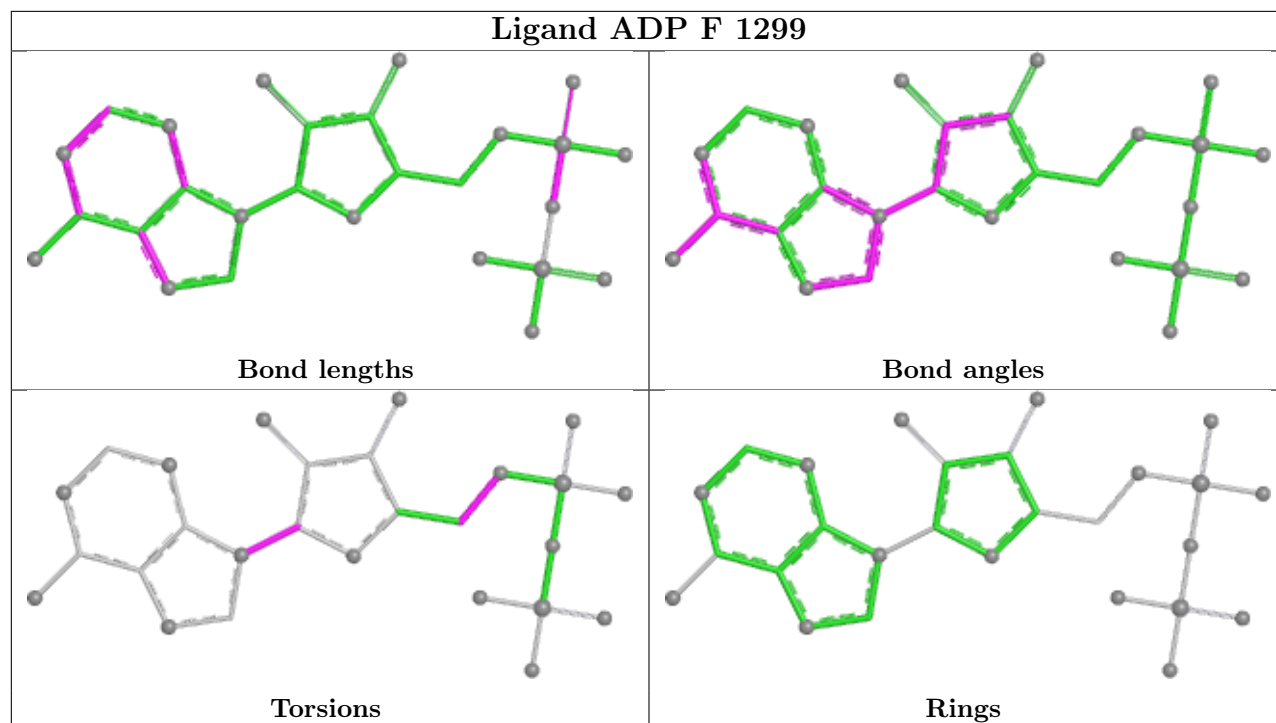












## 5.7 Other polymers [i](#)

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%)	0.05	7 (2%) 59 51	28, 67, 120, 133	0
1	B	297/300 (99%)	-0.11	1 (0%) 90 88	31, 63, 103, 130	0
1	C	299/300 (99%)	-0.39	0 100 100	21, 47, 92, 115	0
1	D	295/300 (98%)	-0.41	1 (0%) 90 88	17, 46, 88, 132	0
1	E	288/300 (96%)	0.23	6 (2%) 63 55	52, 82, 128, 158	0
1	F	292/300 (97%)	0.19	7 (2%) 59 51	45, 90, 139, 157	0
1	G	298/300 (99%)	0.22	5 (1%) 69 62	49, 87, 124, 155	0
1	H	296/300 (98%)	0.56	19 (6%) 25 21	53, 106, 135, 142	0
1	I	289/300 (96%)	0.18	5 (1%) 69 62	45, 84, 123, 147	0
1	J	280/300 (93%)	0.78	23 (8%) 17 15	80, 126, 157, 164	0
1	K	274/300 (91%)	1.08	39 (14%) 6 6	106, 140, 161, 167	0
1	L	294/300 (98%)	0.32	3 (1%) 79 74	69, 102, 131, 151	0
All	All	3494/3600 (97%)	0.22	116 (3%) 49 42	17, 85, 147, 167	0

All (116) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	3	LEU	4.0
1	K	131	ALA	3.8
1	H	37	ASN	3.7
1	H	275	GLY	3.7
1	J	3	LEU	3.6
1	J	214	LEU	3.5
1	K	287	THR	3.4
1	K	242	LEU	3.4
1	A	41	SER	3.4
1	I	38	ALA	3.4
1	K	272	ILE	3.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	K	251	GLY	3.2
1	J	247	THR	3.2
1	J	217	LEU	3.2
1	K	8	ALA	3.2
1	K	283	LEU	3.1
1	H	3	LEU	3.1
1	K	294	LEU	3.1
1	K	293	THR	3.1
1	H	286	PHE	3.0
1	K	3	LEU	3.0
1	A	231	LEU	2.9
1	J	216	LEU	2.9
1	F	96	THR	2.9
1	G	295	ILE	2.8
1	K	295	ILE	2.8
1	H	297	ASN	2.8
1	L	39	MET	2.8
1	F	156	ILE	2.8
1	K	76	LEU	2.8
1	J	36	GLY	2.8
1	J	15	LEU	2.8
1	H	218	THR	2.8
1	K	270	ALA	2.7
1	K	129	LYS	2.7
1	K	9	ALA	2.7
1	K	159	VAL	2.7
1	I	2	THR	2.7
1	K	256	ILE	2.7
1	J	222	GLY	2.7
1	K	41	SER	2.7
1	F	89	MET	2.6
1	H	246	GLY	2.6
1	H	30	LEU	2.6
1	K	49	ALA	2.6
1	G	256	ILE	2.6
1	J	295	ILE	2.6
1	I	68	GLY	2.6
1	H	270	ALA	2.6
1	J	272	ILE	2.5
1	E	40	GLU	2.5
1	J	270	ALA	2.5
1	F	7	ASP	2.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	K	186	GLY	2.5
1	H	216	LEU	2.4
1	J	215	MET	2.4
1	J	220	ILE	2.4
1	J	187	VAL	2.4
1	E	220	ILE	2.4
1	K	134	ILE	2.4
1	K	140	THR	2.4
1	J	79	LEU	2.4
1	H	248	ILE	2.4
1	G	68	GLY	2.4
1	F	105	GLY	2.4
1	I	3	LEU	2.4
1	K	245	ASP	2.3
1	A	37	ASN	2.3
1	J	160	GLY	2.3
1	L	44	LEU	2.3
1	H	22	ILE	2.3
1	I	160	GLY	2.3
1	K	213	LYS	2.2
1	K	225	ASP	2.2
1	A	295	ILE	2.2
1	J	218	THR	2.2
1	K	205	VAL	2.2
1	K	246	GLY	2.2
1	H	214	LEU	2.2
1	J	260	LEU	2.2
1	G	296	SER	2.2
1	E	88	GLY	2.2
1	K	286	PHE	2.2
1	J	283	LEU	2.2
1	H	259	ALA	2.2
1	K	38	ALA	2.2
1	F	158	HIS	2.2
1	E	142	THR	2.2
1	G	39	MET	2.2
1	L	36	GLY	2.2
1	H	223	LEU	2.2
1	K	282	LEU	2.2
1	A	8	ALA	2.2
1	E	244	ALA	2.2
1	H	256	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	297	ASN	2.1
1	H	291	VAL	2.1
1	K	281	VAL	2.1
1	K	115	LEU	2.1
1	J	72	ILE	2.1
1	J	37	ASN	2.1
1	H	217	LEU	2.1
1	K	170	LEU	2.1
1	B	34	TYR	2.1
1	K	22	ILE	2.1
1	K	243	ILE	2.1
1	F	9	ALA	2.1
1	H	293	THR	2.1
1	J	9	ALA	2.1
1	K	83	SER	2.0
1	K	44	LEU	2.0
1	K	135	ARG	2.0
1	J	89	MET	2.0
1	K	79	LEU	2.0
1	A	286	PHE	2.0
1	A	39	MET	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
4	MG	I	1299	1/1	0.59	0.20	74,74,74,74	0
4	MG	C	1301	1/1	0.61	0.12	110,110,110,110	0

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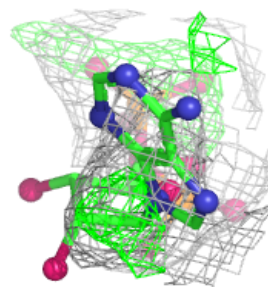
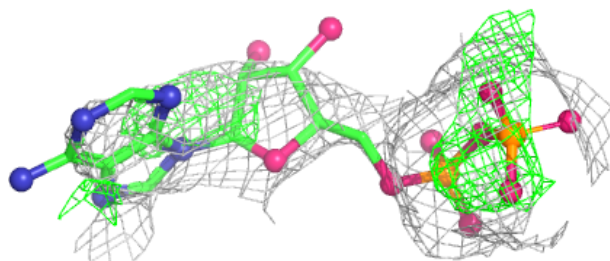
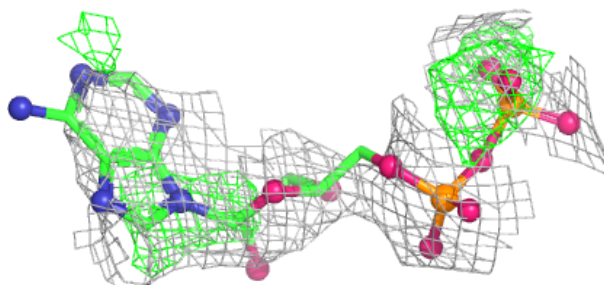
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	NLG	K	1298	13/13	0.65	0.17	100,101,102,103	13
3	ADP	H	1297	27/27	0.72	0.26	120,121,122,122	27
3	ADP	J	1298	27/27	0.73	0.27	123,124,125,125	27
2	NLG	L	1302	13/13	0.76	0.18	108,110,112,112	0
4	MG	L	1301	1/1	0.76	0.28	68,68,68,68	0
3	ADP	C	1300	27/27	0.79	0.13	70,90,117,118	0
4	MG	H	1298	1/1	0.79	0.11	94,94,94,94	0
2	NLG	E	1301	13/13	0.79	0.13	79,83,86,86	0
2	NLG	F	1300	13/13	0.79	0.42	119,119,120,120	13
2	NLG	G	1301	13/13	0.80	0.18	91,95,99,99	13
4	MG	D	1301	1/1	0.82	0.09	56,56,56,56	0
2	NLG	H	1299	13/13	0.83	0.52	115,116,118,118	13
2	NLG	I	1300	13/13	0.85	0.12	93,95,96,96	0
2	NLG	A	1302	13/13	0.86	0.11	75,78,82,82	0
4	MG	E	1300	1/1	0.87	0.26	69,69,69,69	0
3	ADP	G	1299	27/27	0.87	0.10	83,93,120,120	0
5	CL	H	1300	1/1	0.87	0.08	97,97,97,97	0
3	ADP	F	1299	27/27	0.88	0.08	103,109,124,125	0
5	CL	L	1303	1/1	0.90	0.18	100,100,100,100	0
4	MG	G	1300	1/1	0.91	0.08	85,85,85,85	0
2	NLG	D	1302	13/13	0.92	0.11	56,58,61,64	0
5	CL	B	1303	1/1	0.92	0.10	82,82,82,82	0
3	ADP	L	1300	27/27	0.92	0.08	68,76,90,92	0
4	MG	B	1301	1/1	0.92	0.22	50,50,50,50	0
2	NLG	B	1302	13/13	0.93	0.10	57,64,66,68	0
5	CL	G	1302	1/1	0.93	0.12	92,92,92,92	0
3	ADP	I	1298	27/27	0.93	0.09	48,53,82,84	0
3	ADP	E	1299	27/27	0.93	0.09	55,64,77,77	0
3	ADP	B	1300	27/27	0.95	0.07	62,68,71,72	0
3	ADP	D	1300	27/27	0.95	0.07	43,48,58,59	0
5	CL	D	1303	1/1	0.95	0.10	86,86,86,86	0
5	CL	C	1302	1/1	0.96	0.13	84,84,84,84	0

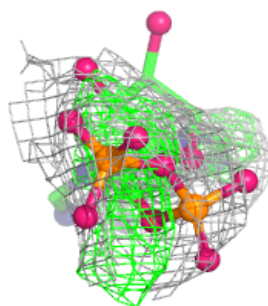
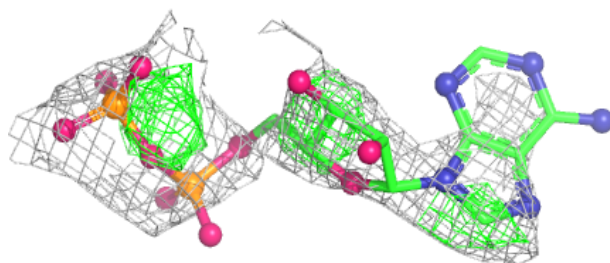
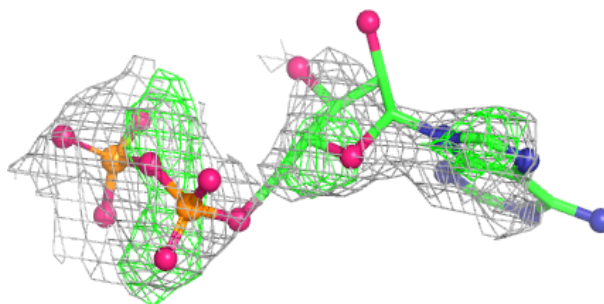
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

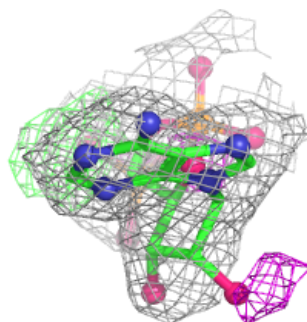
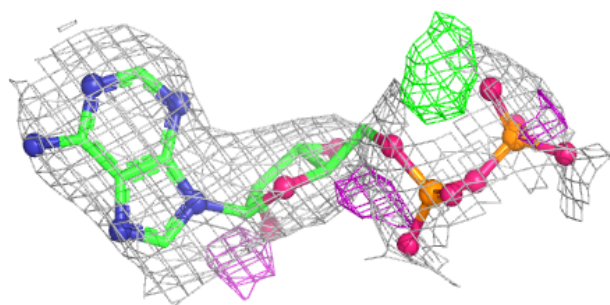
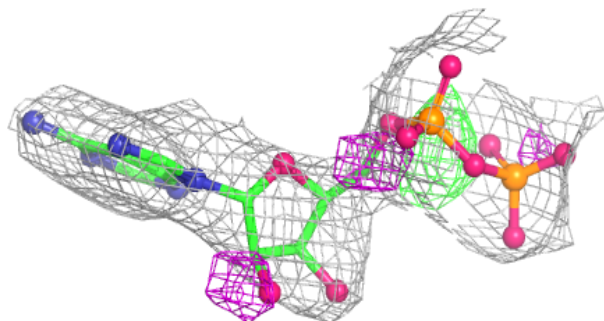
**Electron density around ADP J 1298:**

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

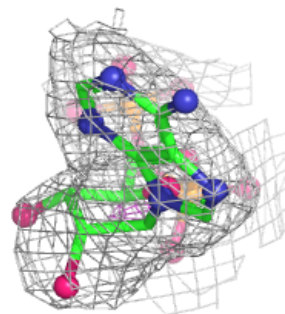
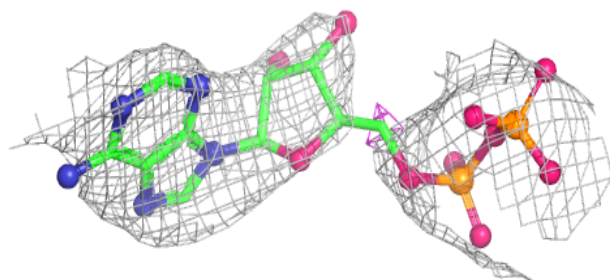
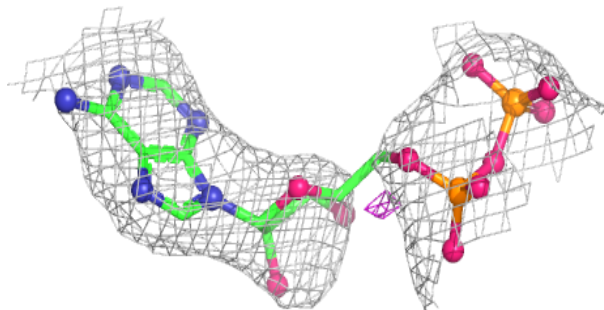


**Electron density around ADP C 1300:**

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

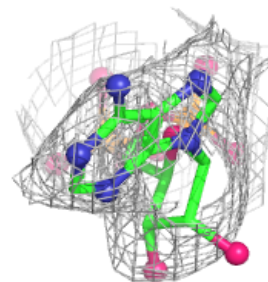
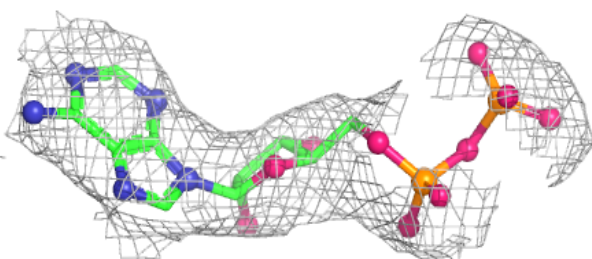
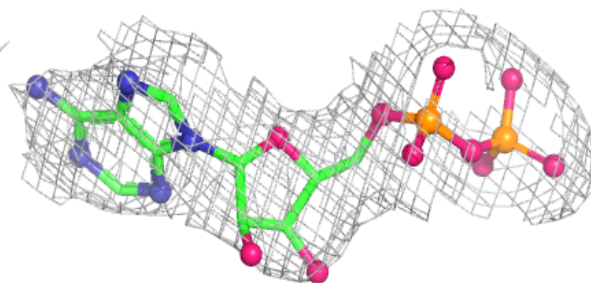
**Electron density around ADP G 1299:**

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

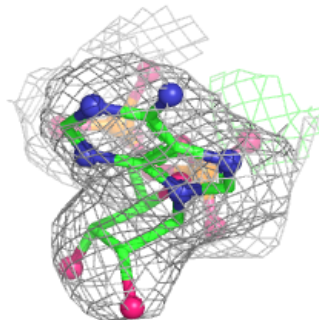
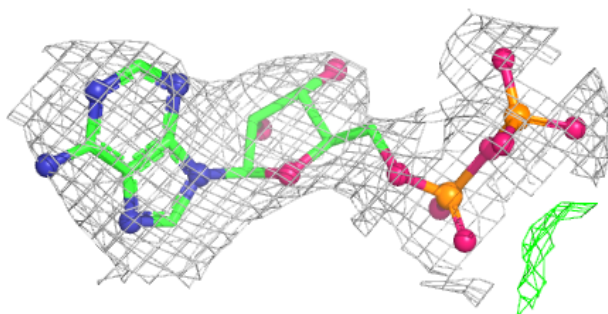
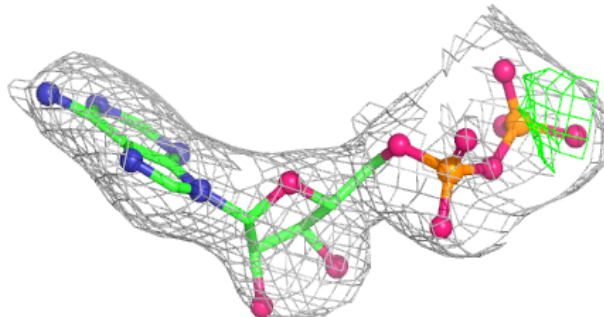


**Electron density around ADP F 1299:**

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

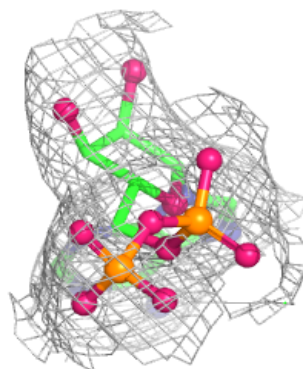
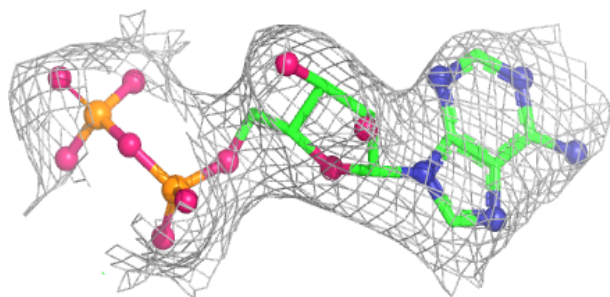
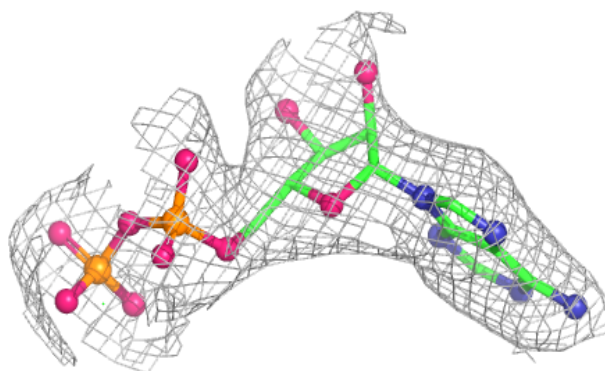
**Electron density around ADP L 1300:**

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

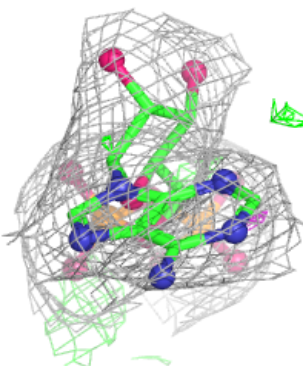
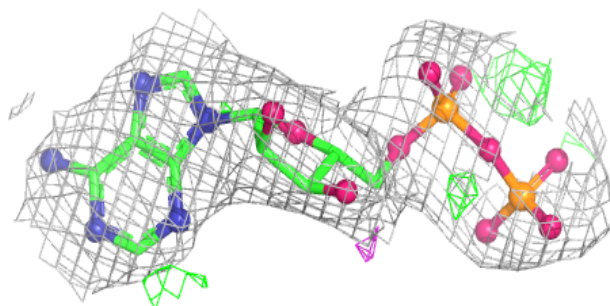
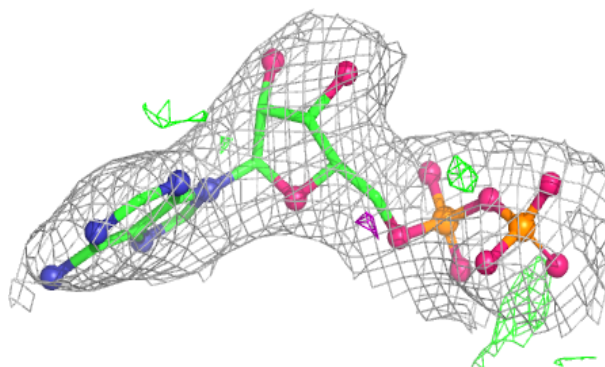


**Electron density around ADP I 1298:**

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

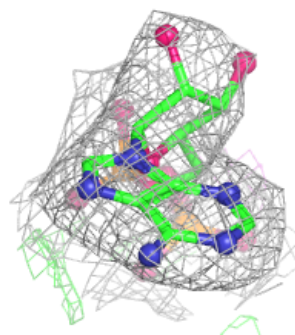
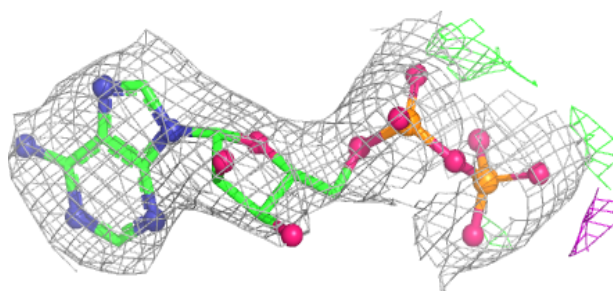
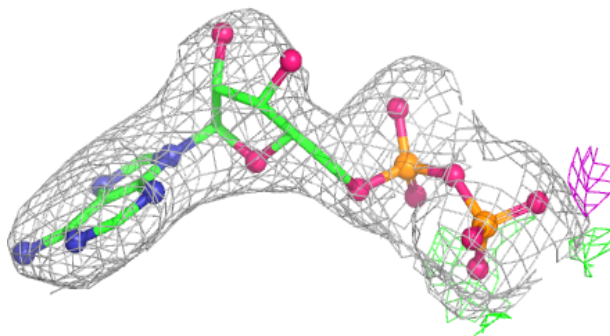
**Electron density around ADP E 1299:**

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

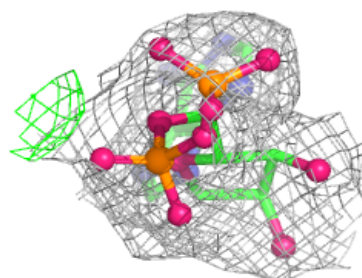
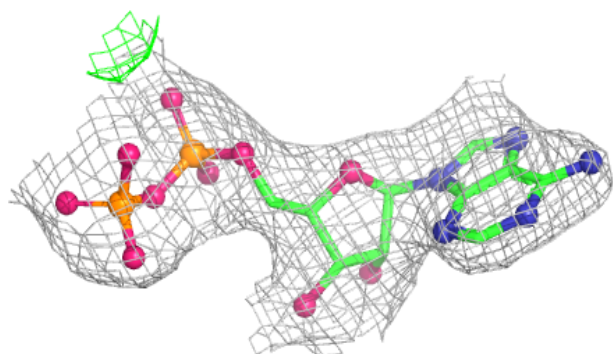
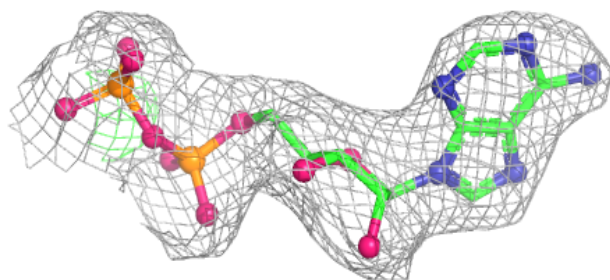


**Electron density around ADP B 1300:**

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

**Electron density around ADP D 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.