



## Full wwPDB X-ray Structure Validation Report ⓘ

Aug 16, 2023 – 01:17 PM EDT

PDB ID : 1ZY8  
Title : The crystal structure of dihydrolipoamide dehydrogenase and dihydrolipoamide dehydrogenase-binding protein (didomain) subcomplex of human pyruvate dehydrogenase complex.  
Authors : Ciszak, E.M.; Makal, A.; Hong, Y.S.; Vettaikorumakankauv, A.K.; Korotchkina, L.G.; Patel, M.S.  
Deposited on : 2005-06-09  
Resolution : 2.59 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](#) ①) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtrriage (Phenix) : 1.13  
EDS : 2.35  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35

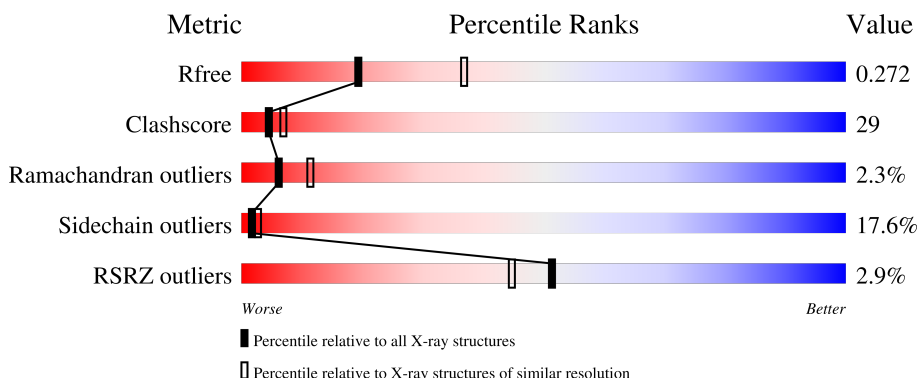
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.59 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	1-A	474	
1	1-B	474	
1	1-C	474	
1	1-D	474	
1	1-E	474	

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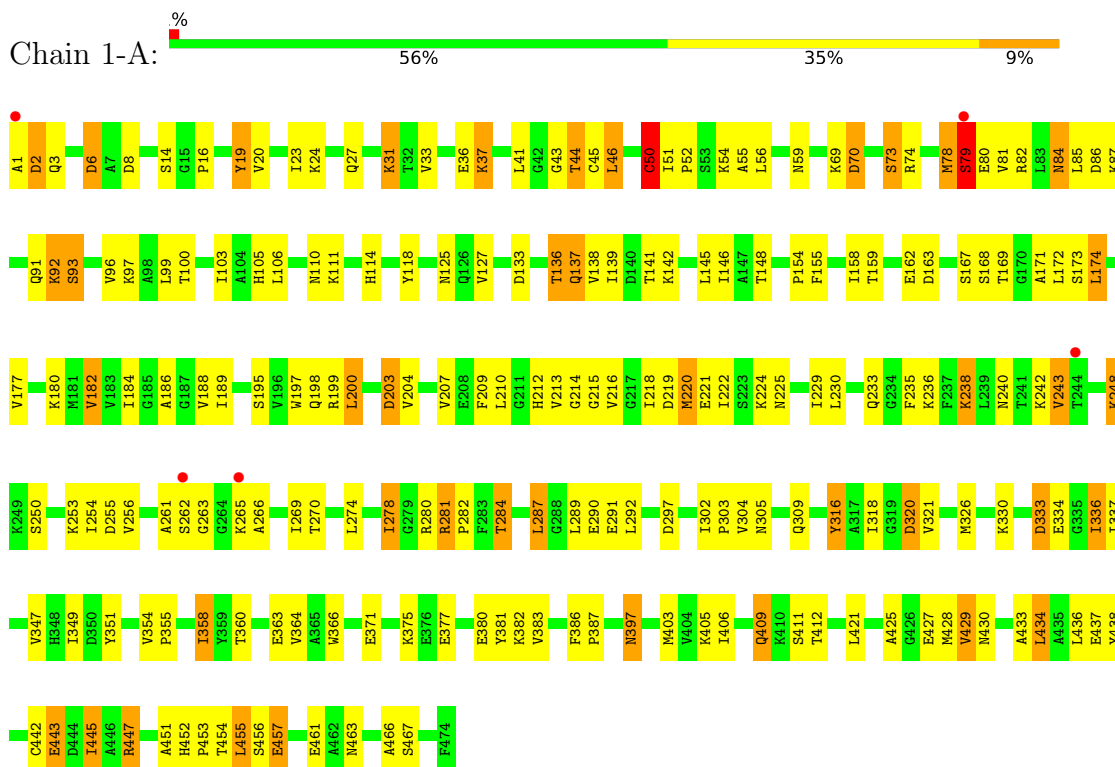
Mol	Chain	Length	Quality of chain
1	1-F	474	% 54% 37% 9%
1	1-G	474	2% 53% 37% 10%
1	1-H	474	% 56% 34% 9%
1	1-I	474	8% 44% 46% 10%
1	1-J	474	3% 49% 38% 12%
1	2-A	474	% 64% 35%
1	2-B	474	% 60% 39%
1	2-C	474	% 62% 37%
1	2-D	474	% 56% 42%
1	2-E	474	% 61% 39%
1	2-F	474	% 62% 37%
1	2-G	474	2% 59% 40%
1	2-H	474	% 63% 36%
1	2-I	474	8% 50% 48%
1	2-J	474	3% 58% 41%
2	1-K	229	12% 81%
2	1-L	229	6% 8% 8% 81%
2	1-M	229	5% 10% 81%
2	1-N	229	11% 13% 81%
2	1-O	229	8% 7% 10% 81%
2	2-K	229	11% 6% 10% 82%
2	2-L	229	5% 6% 12% 82%
2	2-M	229	5% 14% 81%
2	2-N	229	10% 5% 11% 82%
2	2-O	229	100%

ENTRY-COMPOSITION INFOmissingINFO

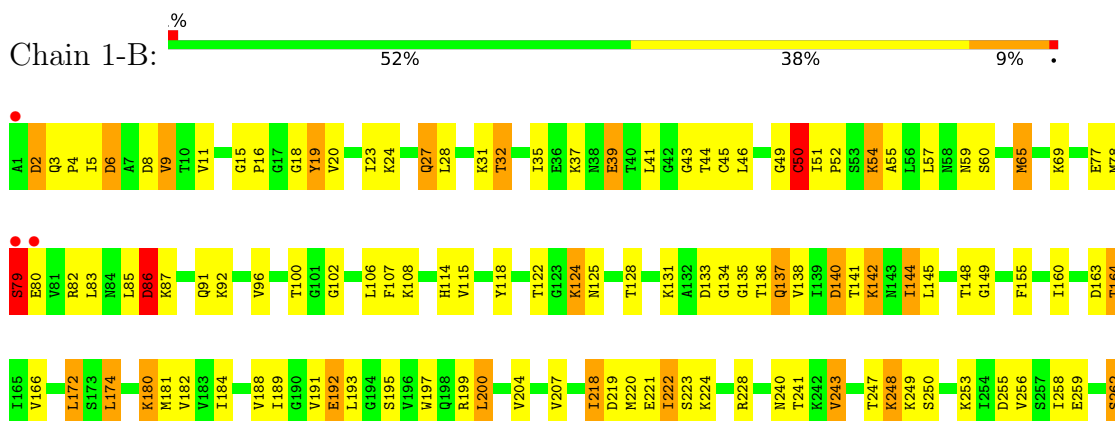
## 2 Residue-property plots [i](#)

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

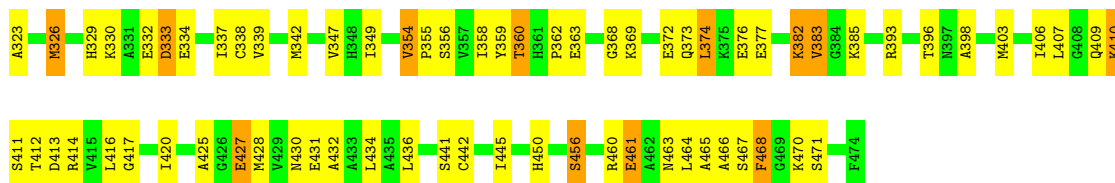
- Molecule 1: Dihydrolipoyl dehydrogenase, mitochondrial



- Molecule 1: Dihydrolipoyl dehydrogenase, mitochondrial

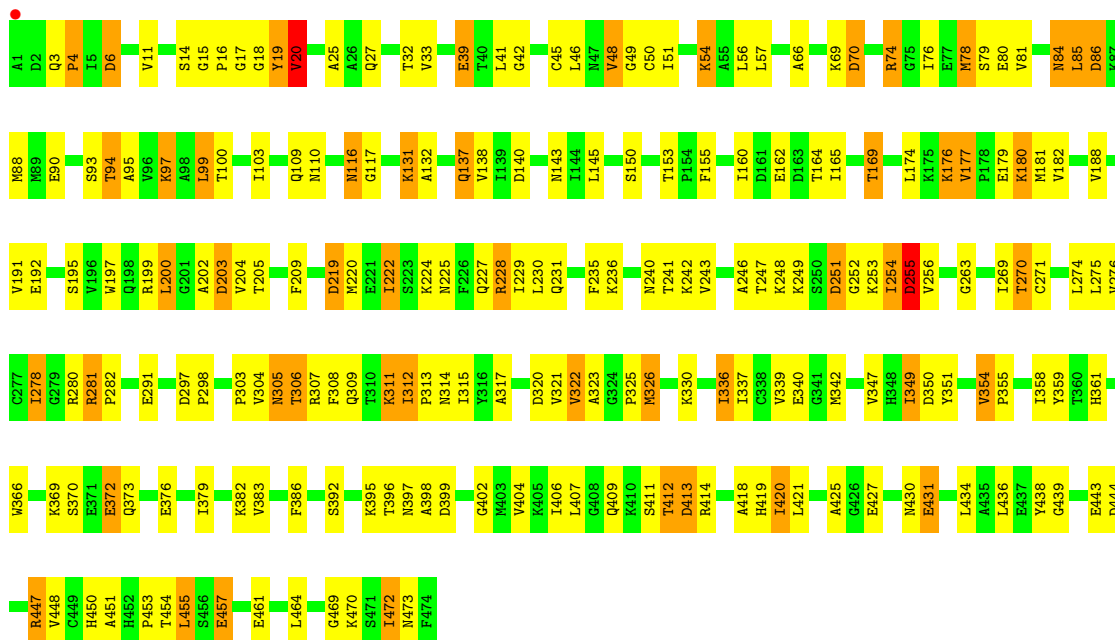






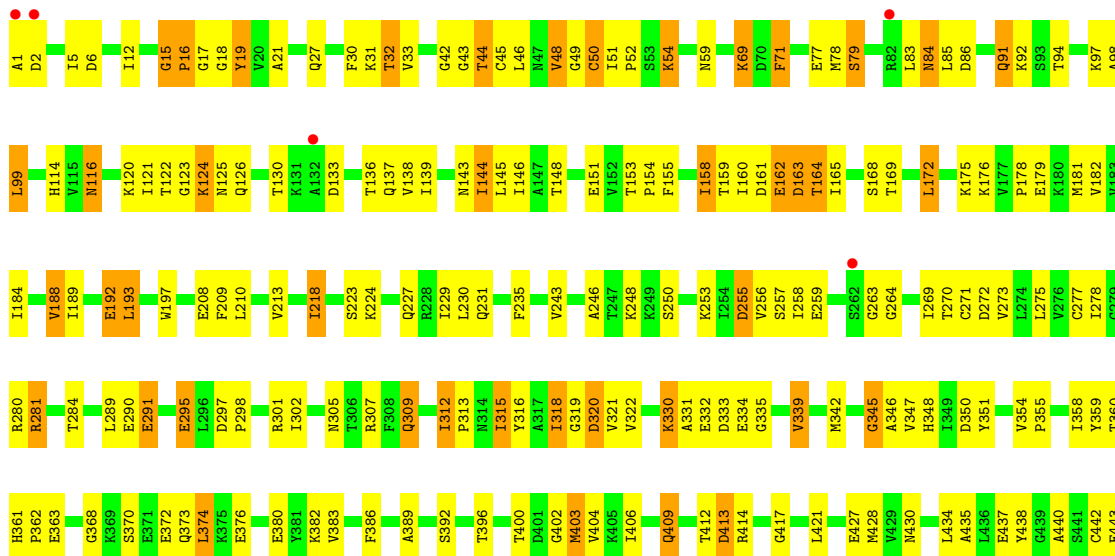
• Molecule 1: Dihydrolipoyl dehydrogenase, mitochondrial

Chain 1-E: 55% 34% 11%



• Molecule 1: Dihydrolipoyl dehydrogenase, mitochondrial

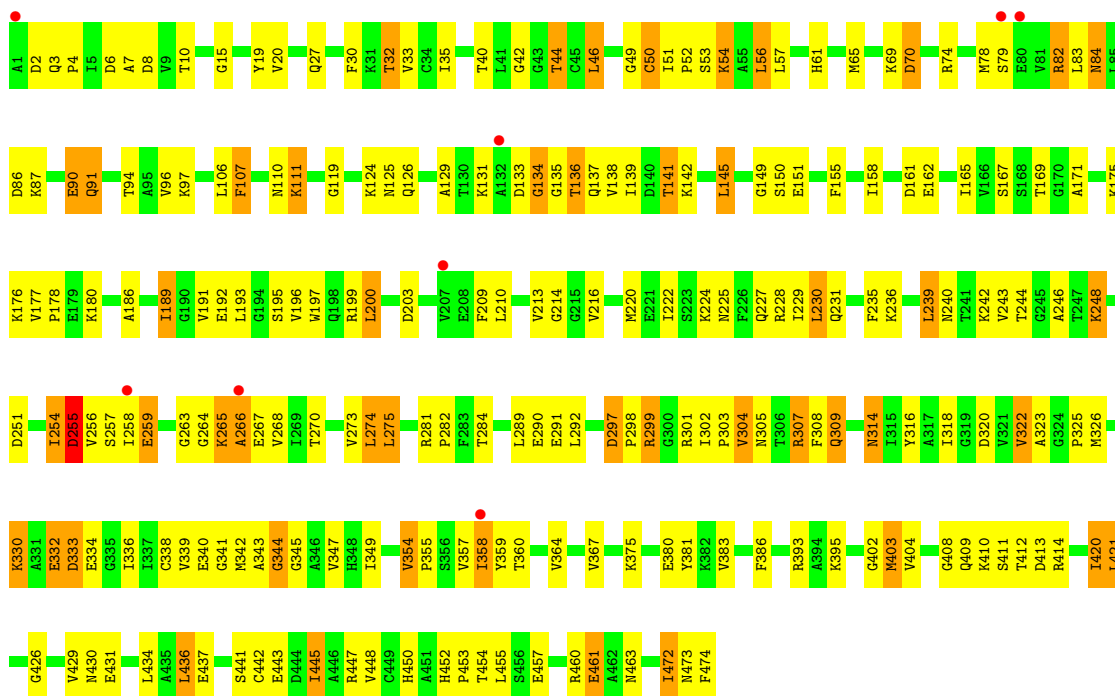
Chain 1-F: 54% 37% 9%



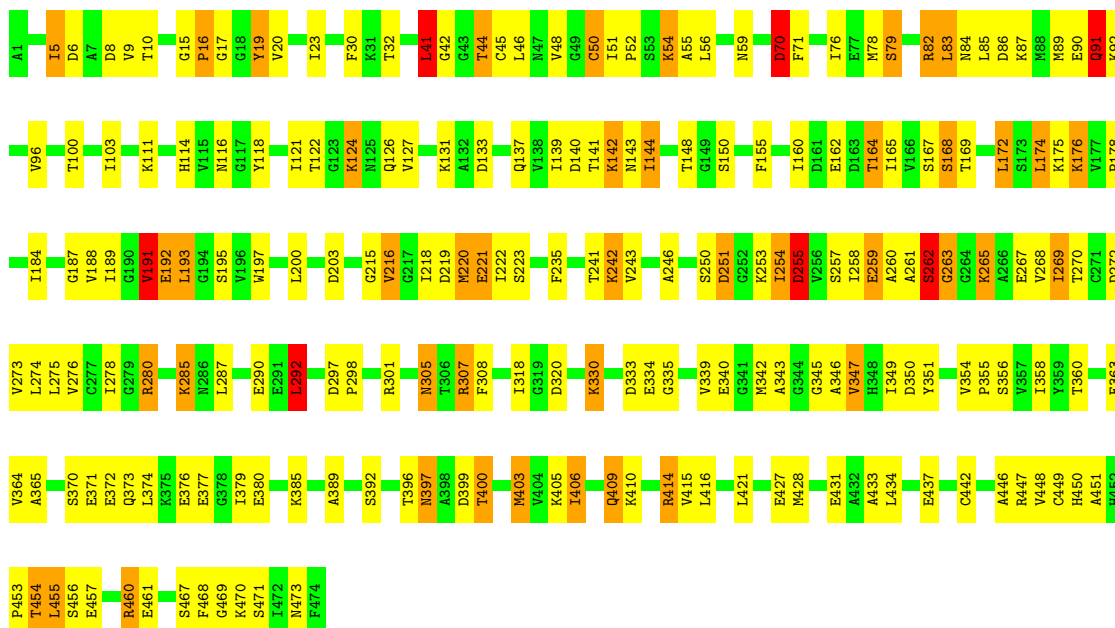




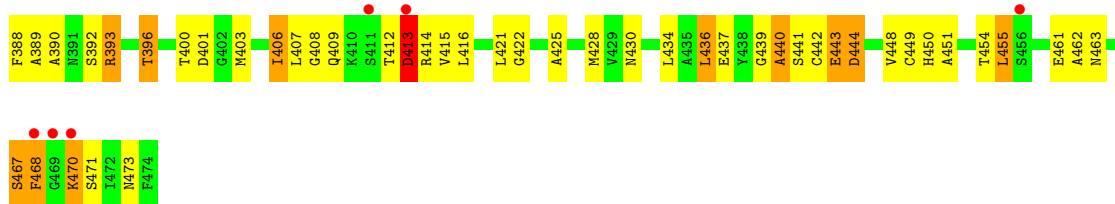
● Molecule 1: Dihydrolipoyl dehydrogenase, mitochondrial



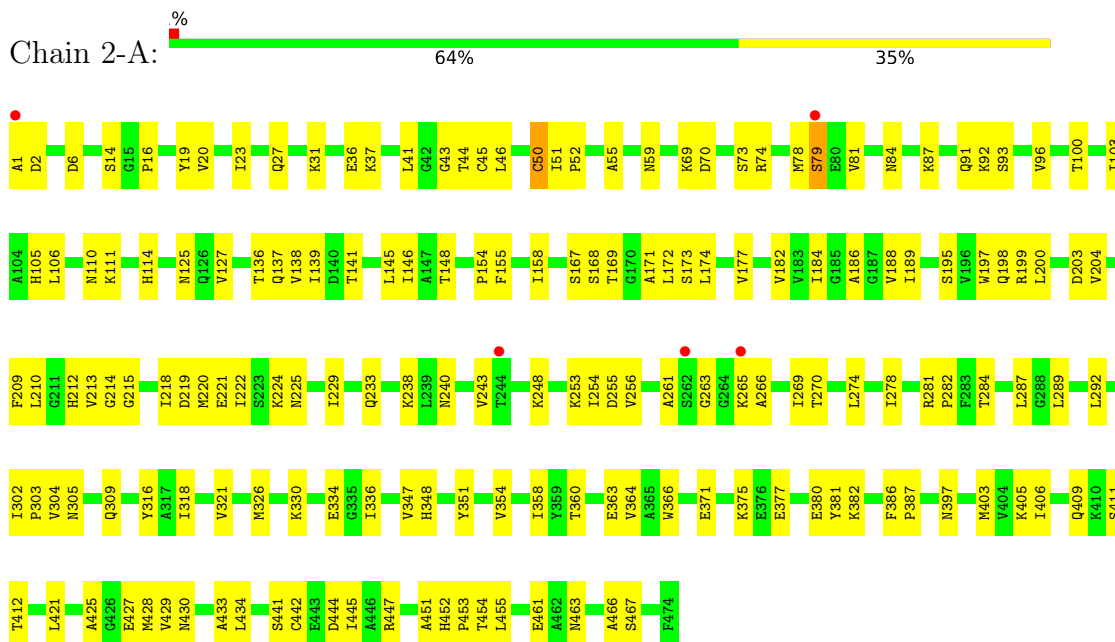
● Molecule 1: Dihydrolipoyl dehydrogenase, mitochondrial



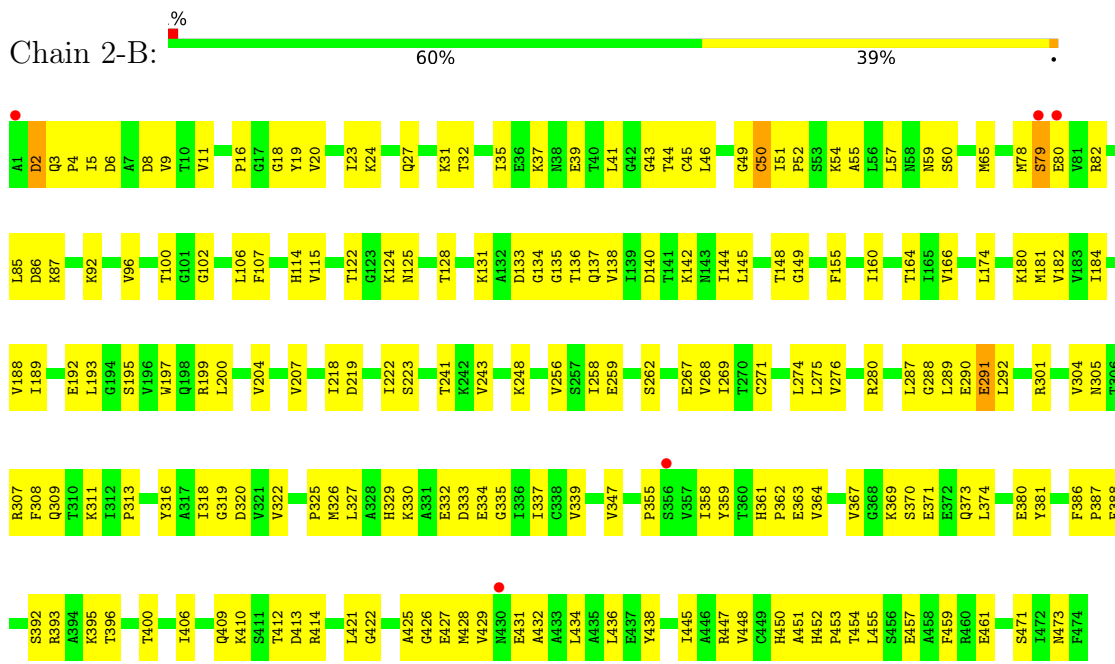




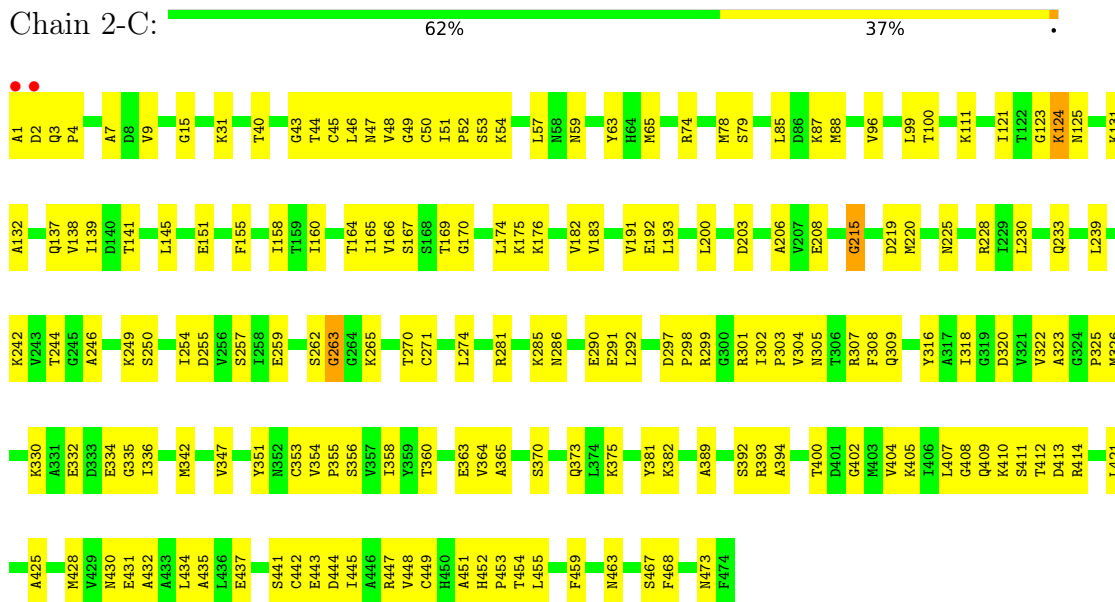
● Molecule 1: Dihydrolipoyl dehydrogenase, mitochondrial



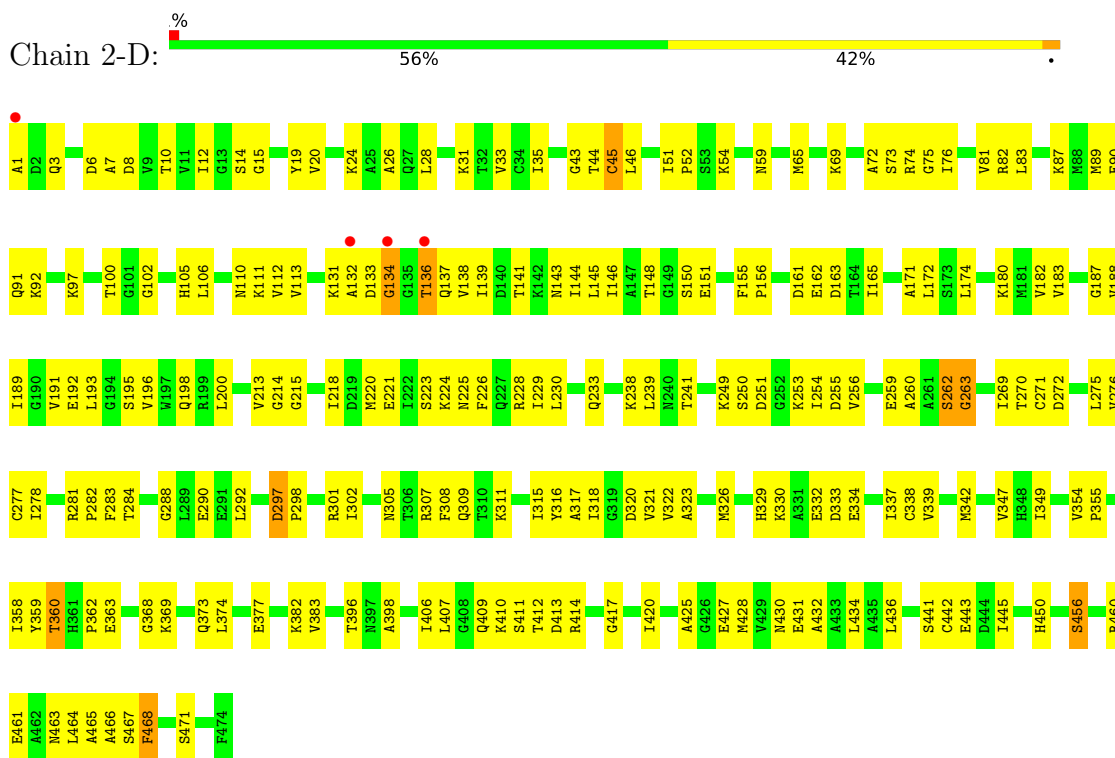
● Molecule 1: Dihydrolipoyl dehydrogenase, mitochondrial



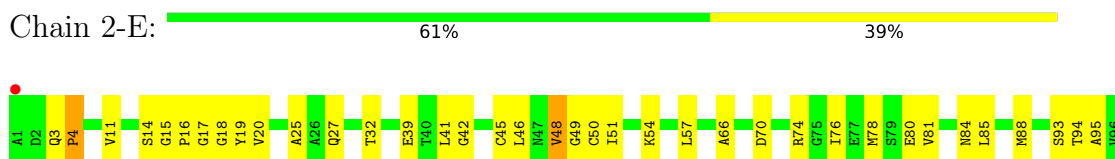
● Molecule 1: Dihydrolipoyl dehydrogenase, mitochondrial

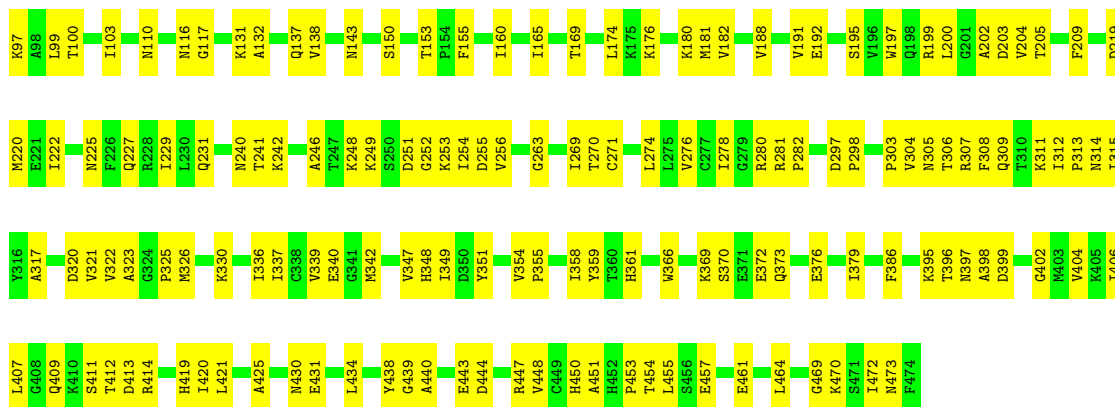


• Molecule 1: Dihydropolyl dehydrogenase, mitochondrial

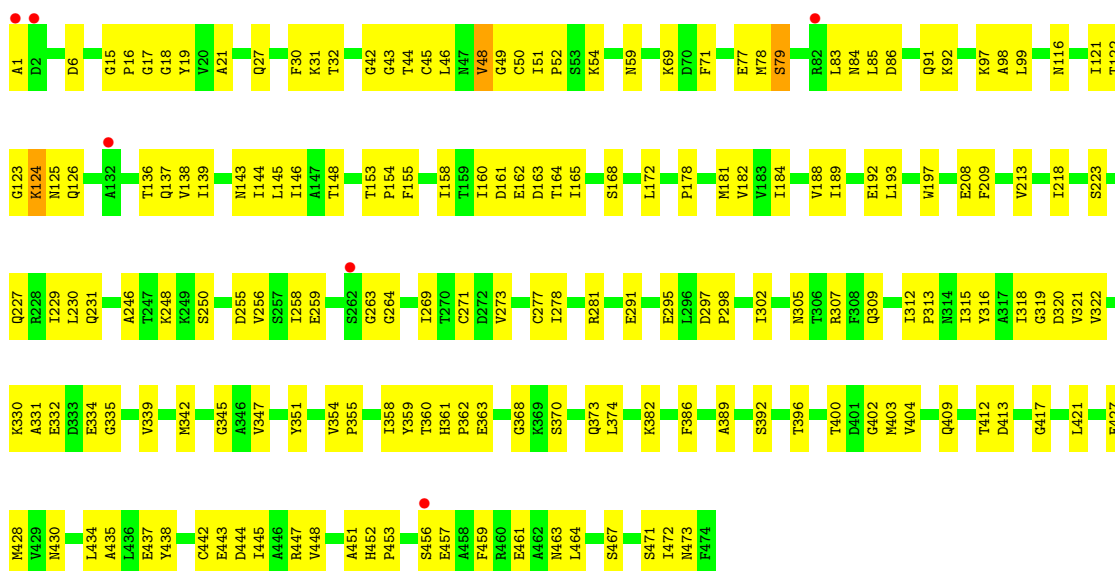


• Molecule 1: Dihydropolyl dehydrogenase, mitochondrial

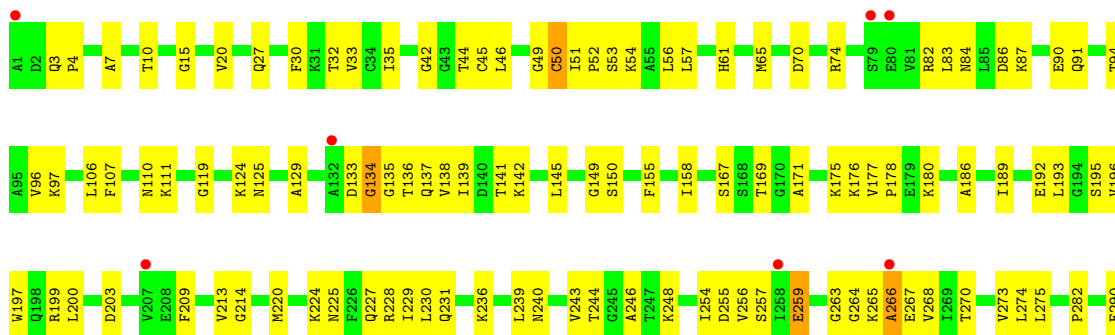


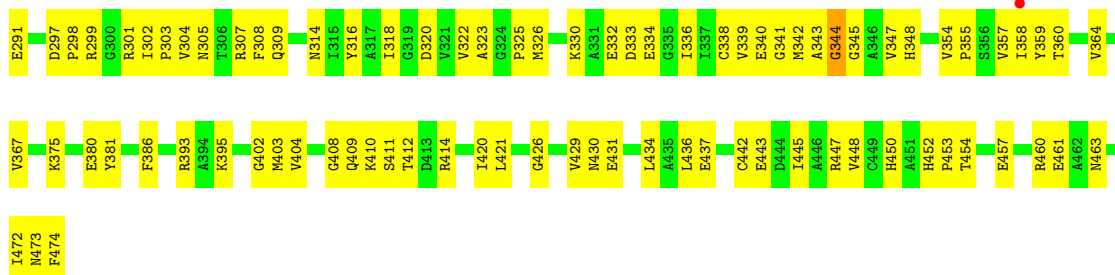


● Molecule 1: Dihydrolipoyl dehydrogenase, mitochondrial

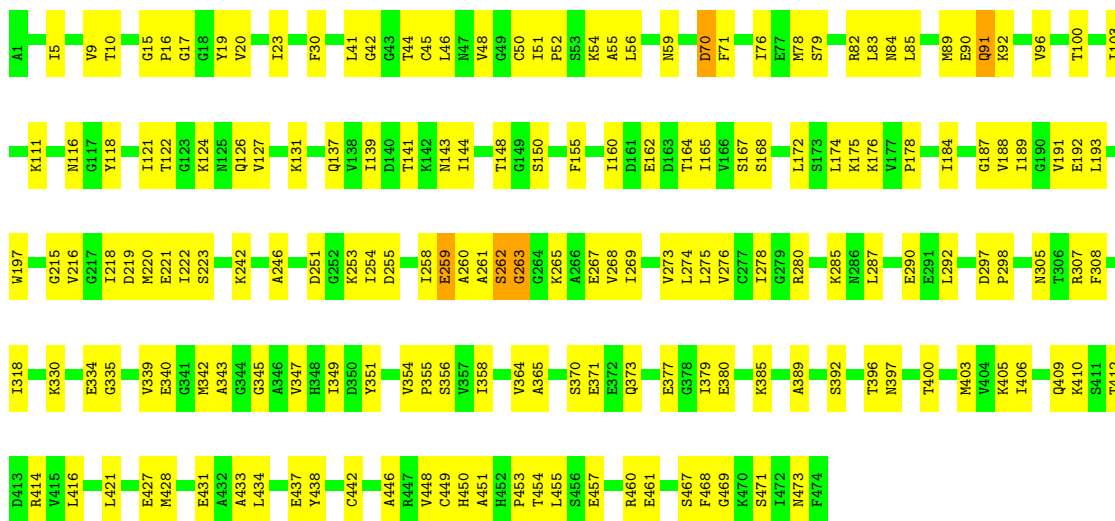


● Molecule 1: Dihydrolipoyl dehydrogenase, mitochondrial

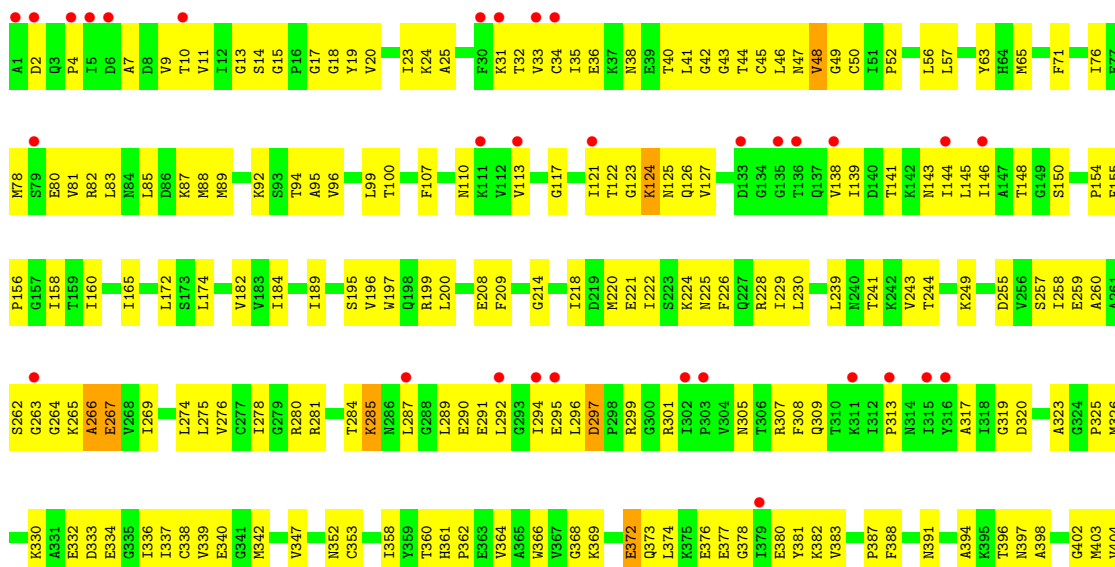


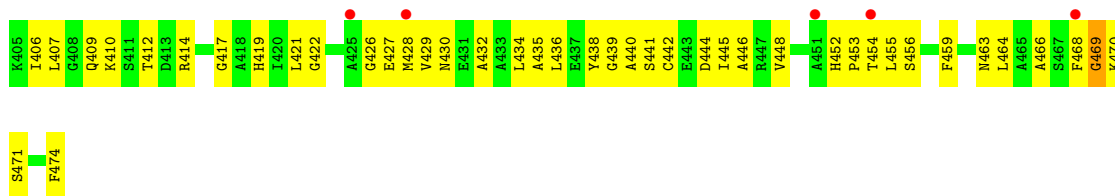


• Molecule 1: Dihydrolipoyl dehydrogenase, mitochondrial

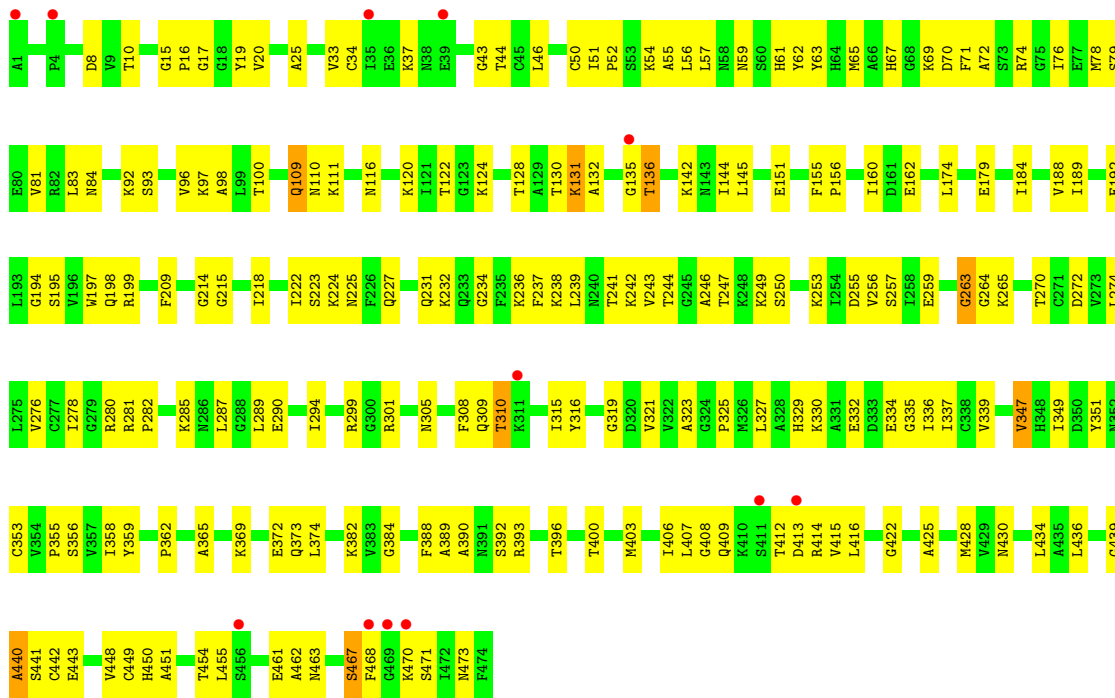


• Molecule 1: Dihydrolipoyl dehydrogenase, mitochondrial

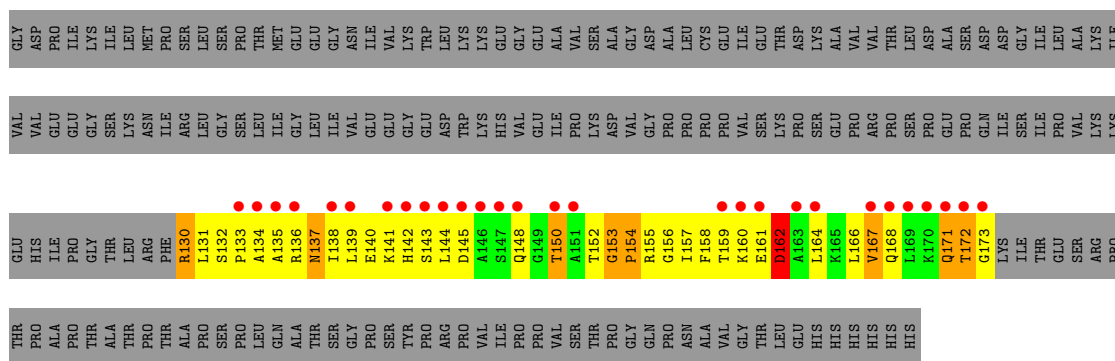




• Molecule 1: Dihydrolipoyl dehydrogenase, mitochondrial

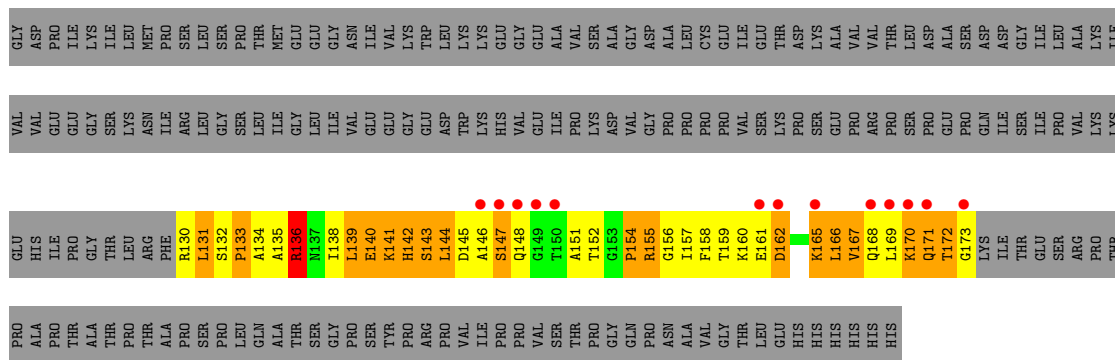


• Molecule 2: Pyruvate dehydrogenase protein X component, mitochondrial

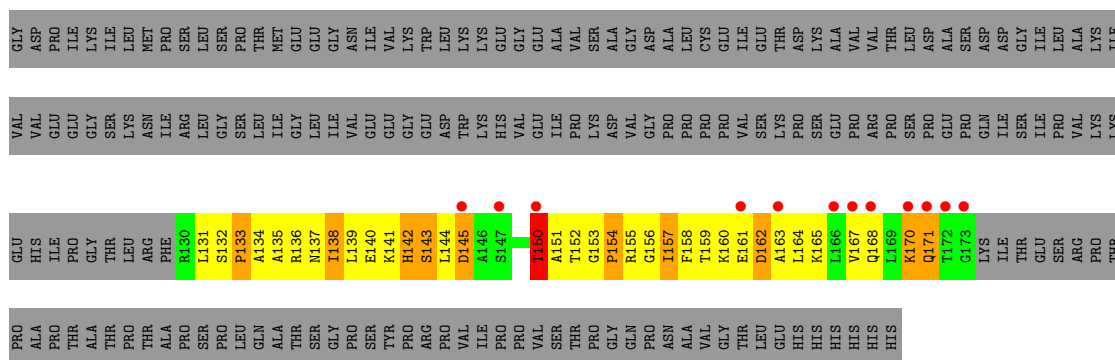


• Molecule 2: Pyruvate dehydrogenase protein X component, mitochondrial

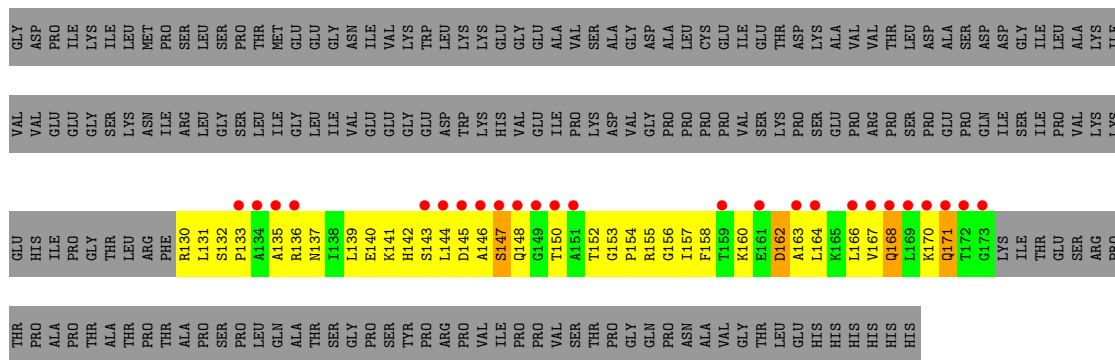




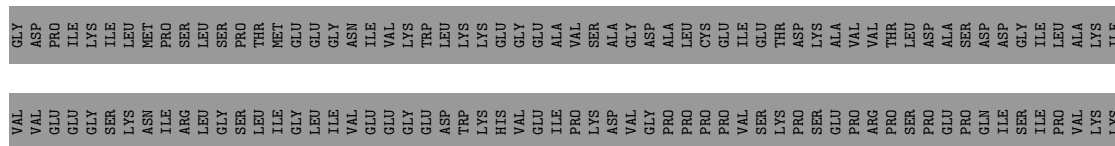
• Molecule 2: Pyruvate dehydrogenase protein X component, mitochondrial



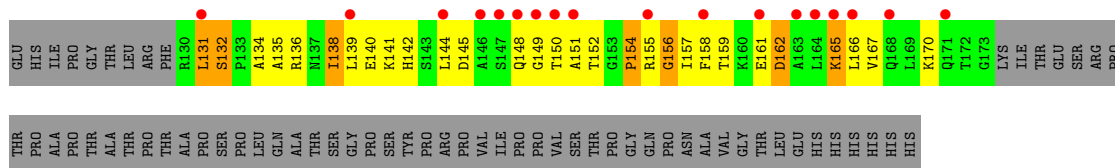
• Molecule 2: Pyruvate dehydrogenase protein X component, mitochondrial



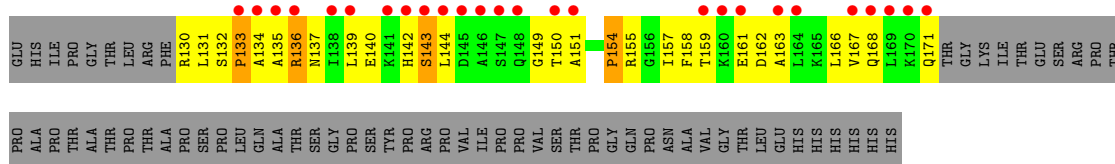
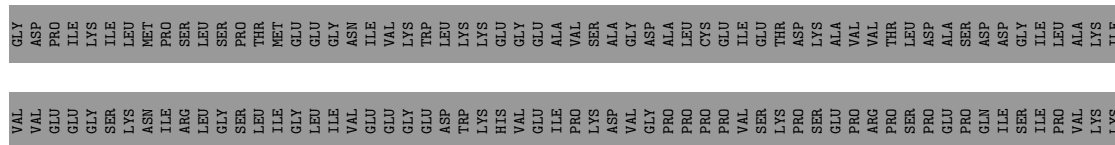
• Molecule 2: Pyruvate dehydrogenase protein X component, mitochondrial



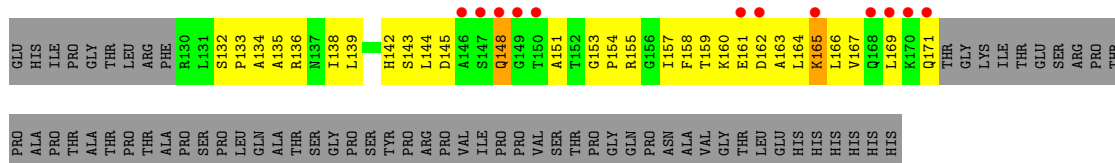
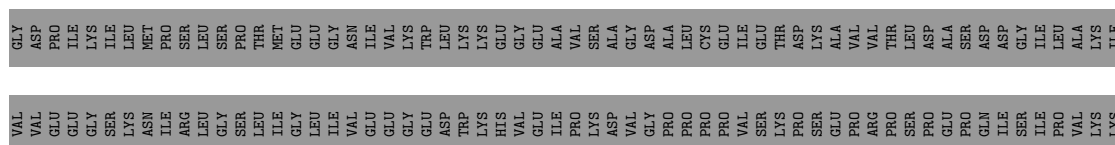




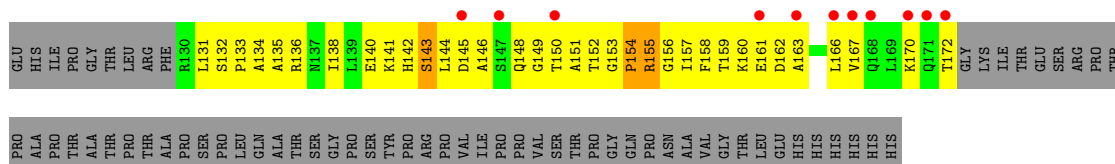
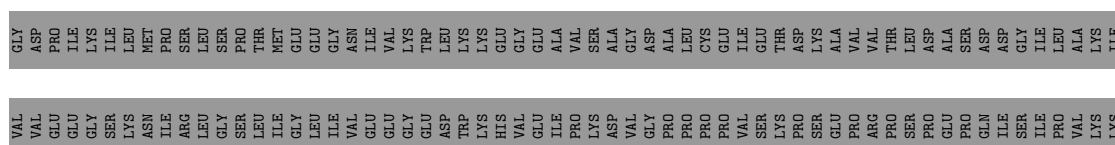
• Molecule 2: Pyruvate dehydrogenase protein X component, mitochondrial



• Molecule 2: Pyruvate dehydrogenase protein X component, mitochondrial



• Molecule 2: Pyruvate dehydrogenase protein X component, mitochondrial





### 3 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	168.79Å 186.91Å 217.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.64 – 2.59 45.52 – 2.59	Depositor EDS
% Data completeness (in resolution range)	88.5 (45.64-2.59) 78.1 (45.52-2.59)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.32 (at 2.58Å)	Xtrriage
Refinement program	REFMAC 5.1.19, CNS	Depositor
R, $R_{free}$	0.208 , 0.276 0.205 , 0.272	Depositor DCC
$R_{free}$ test set	9410 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	34.2	Xtrriage
Anisotropy	0.649	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 44.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	75406	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.04% 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.

## 4 Model quality i

### 4.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: FAD

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	1-A	1.10	5/3581 (0.1%)	1.08	15/4836 (0.3%)
1	1-B	1.08	6/3581 (0.2%)	1.09	10/4836 (0.2%)
1	1-C	1.17	6/3581 (0.2%)	1.14	16/4836 (0.3%)
1	1-D	1.06	6/3581 (0.2%)	1.11	11/4836 (0.2%)
1	1-E	1.16	10/3581 (0.3%)	1.13	13/4836 (0.3%)
1	1-F	1.10	4/3581 (0.1%)	1.08	14/4836 (0.3%)
1	1-G	1.02	5/3581 (0.1%)	1.05	9/4836 (0.2%)
1	1-H	1.29	7/3581 (0.2%)	1.15	21/4836 (0.4%)
1	1-I	0.87	2/3581 (0.1%)	0.98	14/4836 (0.3%)
1	1-J	0.88	2/3581 (0.1%)	0.98	11/4836 (0.2%)
2	1-K	0.66	0/334	0.93	2/448 (0.4%)
2	1-L	0.66	0/334	0.87	1/448 (0.2%)
2	1-M	0.63	0/334	0.95	2/448 (0.4%)
2	1-N	0.65	0/334	0.88	1/448 (0.2%)
2	1-O	0.67	0/334	0.86	0/448
All	All	1.06	53/37480 (0.1%)	1.07	140/50600 (0.3%)

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
2	1-L	0	1
2	2-K	0	1
All	All	0	2

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1-H	50[A]	CYS	CB-SG	-28.00	1.34	1.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1-H	50[B]	CYS	CB-SG	-28.00	1.34	1.82
1	1-A	50[A]	CYS	CB-SG	-18.52	1.50	1.82
1	1-A	50[B]	CYS	CB-SG	-18.52	1.50	1.82
1	1-F	50[A]	CYS	CB-SG	-18.37	1.51	1.82
1	1-F	50[B]	CYS	CB-SG	-18.37	1.51	1.82
1	1-G	50[A]	CYS	CB-SG	-16.71	1.53	1.82
1	1-G	50[B]	CYS	CB-SG	-16.71	1.53	1.82
1	1-E	50[A]	CYS	CB-SG	-14.74	1.57	1.82
1	1-E	50[B]	CYS	CB-SG	-14.74	1.57	1.82
1	1-B	50[A]	CYS	CB-SG	-13.80	1.58	1.82
1	1-B	50[B]	CYS	CB-SG	-13.80	1.58	1.82
1	1-I	50[A]	CYS	CB-SG	-12.68	1.60	1.82
1	1-I	50[B]	CYS	CB-SG	-12.68	1.60	1.82
1	1-C	50[A]	CYS	CB-SG	-12.23	1.61	1.82
1	1-C	50[B]	CYS	CB-SG	-12.23	1.61	1.82
1	1-D	50[A]	CYS	CB-SG	-10.72	1.64	1.82
1	1-D	50[B]	CYS	CB-SG	-10.72	1.64	1.82
1	1-J	50[A]	CYS	CB-SG	9.17	1.97	1.82
1	1-J	50[B]	CYS	CB-SG	9.17	1.97	1.82
1	1-A	220[A]	MET	SD-CE	8.10	2.23	1.77
1	1-F	192[A]	GLU	CD-OE1	6.89	1.33	1.25
1	1-C	220[A]	MET	SD-CE	6.55	2.14	1.77
1	1-E	322[A]	VAL	CB-CG1	-6.31	1.39	1.52
1	1-B	192[A]	GLU	CD-OE1	6.28	1.32	1.25
1	1-E	20[A]	VAL	CB-CG2	-6.21	1.39	1.52
1	1-D	326[A]	MET	SD-CE	6.03	2.11	1.77
1	1-A	182[A]	VAL	CB-CG2	-5.95	1.40	1.52
1	1-H	220[A]	MET	SD-CE	5.84	2.10	1.77
1	1-E	418[A]	ALA	CA-CB	-5.83	1.40	1.52
1	1-E	457[A]	GLU	CD-OE1	5.70	1.31	1.25
1	1-C	224[A]	LYS	CD-CE	5.62	1.65	1.51
1	1-F	403[A]	MET	SD-CE	5.58	2.09	1.77
1	1-C	326[A]	MET	SD-CE	5.48	2.08	1.77
1	1-A	457[A]	GLU	CD-OE2	5.43	1.31	1.25
1	1-H	221[A]	GLU	CD-OE2	5.42	1.31	1.25
1	1-H	191[A]	VAL	CB-CG1	-5.41	1.41	1.52
1	1-B	65[A]	MET	SD-CE	5.39	2.08	1.77
1	1-G	216[A]	VAL	CB-CG2	5.35	1.64	1.52
1	1-D	461[A]	GLU	CG-CD	5.34	1.59	1.51
1	1-C	180[A]	LYS	CD-CE	5.33	1.64	1.51
1	1-G	332[A]	GLU	CD-OE2	5.29	1.31	1.25
1	1-D	98[A]	ALA	CA-CB	-5.29	1.41	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1-E	177[A]	VAL	CB-CG1	-5.27	1.41	1.52
1	1-H	192[A]	GLU	CD-OE2	5.26	1.31	1.25
1	1-H	142[A]	LYS	CD-CE	5.18	1.64	1.51
1	1-B	340[A]	GLU	CD-OE1	5.17	1.31	1.25
1	1-B	191[A]	VAL	CB-CG2	-5.17	1.42	1.52
1	1-D	461[A]	GLU	CD-OE1	5.15	1.31	1.25
1	1-G	461[A]	GLU	CG-CD	5.10	1.59	1.51
1	1-E	431[A]	GLU	CD-OE2	5.06	1.31	1.25
1	1-E	372[A]	GLU	CD-OE1	5.02	1.31	1.25
1	1-E	228[A]	ARG	CG-CD	5.01	1.64	1.51

All (140) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1-D	50[A]	CYS	CA-CB-SG	11.63	134.94	114.00
1	1-D	50[B]	CYS	CA-CB-SG	11.63	134.94	114.00
1	1-I	203[A]	ASP	CB-CG-OD2	10.15	127.44	118.30
1	1-H	50[A]	CYS	CA-CB-SG	9.38	130.88	114.00
1	1-H	50[B]	CYS	CA-CB-SG	9.38	130.88	114.00
1	1-H	203[A]	ASP	CB-CG-OD2	8.65	126.08	118.30
1	1-A	320[A]	ASP	CB-CG-OD2	8.17	125.65	118.30
1	1-G	333[A]	ASP	CB-CG-OD2	8.13	125.62	118.30
1	1-A	280[A]	ARG	NE-CZ-NH1	-7.99	116.30	120.30
1	1-C	255[A]	ASP	CB-CG-OD2	7.85	125.36	118.30
1	1-I	86[A]	ASP	CB-CG-OD2	7.74	125.27	118.30
1	1-E	444[A]	ASP	CB-CG-OD2	7.55	125.09	118.30
1	1-G	70[A]	ASP	CB-CG-OD2	7.36	124.92	118.30
1	1-H	70[A]	ASP	CB-CG-OD2	7.35	124.92	118.30
1	1-C	219[A]	ASP	CB-CG-OD2	7.25	124.83	118.30
1	1-F	163[A]	ASP	CB-CG-OD2	7.20	124.78	118.30
1	1-I	251[A]	ASP	CB-CG-OD2	7.14	124.72	118.30
1	1-F	333[A]	ASP	CB-CG-OD2	7.11	124.70	118.30
1	1-G	50[A]	CYS	CA-CB-SG	7.07	126.73	114.00
1	1-G	50[B]	CYS	CA-CB-SG	7.07	126.73	114.00
1	1-E	255[A]	ASP	CB-CG-OD1	7.05	124.64	118.30
1	1-C	50[A]	CYS	CA-CB-SG	7.03	126.66	114.00
1	1-C	50[B]	CYS	CA-CB-SG	7.03	126.66	114.00
1	1-G	161[A]	ASP	CB-CG-OD2	7.03	124.63	118.30
1	1-H	86[A]	ASP	CB-CG-OD2	6.99	124.59	118.30
1	1-C	163[A]	ASP	CB-CG-OD2	6.99	124.59	118.30
1	1-D	219[A]	ASP	CB-CG-OD2	6.97	124.57	118.30
1	1-A	455[A]	LEU	CB-CG-CD2	-6.94	99.20	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1-I	272[A]	ASP	CB-CG-OD2	6.91	124.52	118.30
1	1-E	86[A]	ASP	CB-CG-OD2	6.88	124.49	118.30
1	1-H	399[A]	ASP	CB-CG-OD2	6.87	124.48	118.30
1	1-H	6[A]	ASP	CB-CG-OD2	6.87	124.48	118.30
1	1-A	8[A]	ASP	CB-CG-OD2	6.84	124.45	118.30
1	1-J	444[A]	ASP	CB-CG-OD2	6.75	124.38	118.30
1	1-E	140[A]	ASP	CB-CG-OD2	6.67	124.30	118.30
1	1-H	280[A]	ARG	NE-CZ-NH2	-6.66	116.97	120.30
1	1-J	272[A]	ASP	CB-CG-OD2	6.66	124.29	118.30
1	1-J	255[A]	ASP	CB-CG-OD2	6.64	124.28	118.30
1	1-D	8[A]	ASP	CB-CG-OD2	6.56	124.21	118.30
1	1-A	133[A]	ASP	CB-CG-OD2	6.55	124.20	118.30
1	1-G	251[A]	ASP	CB-CG-OD2	6.55	124.19	118.30
1	1-E	203[A]	ASP	CB-CG-OD2	6.55	124.19	118.30
1	1-H	320[A]	ASP	CB-CG-OD2	6.50	124.15	118.30
2	1-M	162[A]	ASP	CB-CG-OD2	6.46	124.12	118.30
1	1-H	16[A]	PRO	C-N-CA	-6.43	108.79	122.30
1	1-B	447[A]	ARG	NE-CZ-NH1	6.43	123.51	120.30
1	1-H	140[A]	ASP	CB-CG-OD2	6.37	124.03	118.30
1	1-H	251[A]	ASP	CB-CG-OD2	6.36	124.02	118.30
2	1-L	162[A]	ASP	CB-CG-OD2	6.33	124.00	118.30
1	1-A	70[A]	ASP	CB-CG-OD2	6.31	123.98	118.30
1	1-D	6[A]	ASP	CB-CG-OD2	6.31	123.98	118.30
1	1-I	444[A]	ASP	CB-CG-OD2	6.30	123.97	118.30
1	1-F	50[A]	CYS	CA-CB-SG	6.29	125.32	114.00
1	1-F	50[B]	CYS	CA-CB-SG	6.29	125.32	114.00
1	1-H	8[A]	ASP	CB-CG-OD2	6.29	123.96	118.30
1	1-H	280[A]	ARG	NE-CZ-NH1	6.27	123.44	120.30
1	1-H	292[A]	LEU	CA-CB-CG	6.26	129.70	115.30
1	1-J	413[A]	ASP	CB-CG-OD2	6.21	123.89	118.30
1	1-G	255[A]	ASP	CB-CG-OD2	6.20	123.88	118.30
1	1-E	251[A]	ASP	CB-CG-OD2	6.19	123.88	118.30
1	1-C	350[A]	ASP	CB-CG-OD2	6.17	123.85	118.30
1	1-G	8[A]	ASP	CB-CG-OD2	6.13	123.82	118.30
1	1-J	86[A]	ASP	CB-CG-OD2	6.11	123.80	118.30
1	1-H	350[A]	ASP	CB-CG-OD2	6.07	123.76	118.30
1	1-D	133[A]	ASP	CB-CG-OD2	6.07	123.76	118.30
1	1-I	163[A]	ASP	CB-CG-OD2	6.04	123.73	118.30
1	1-B	172[A]	LEU	CA-CB-CG	5.99	129.07	115.30
1	1-H	333[A]	ASP	CB-CG-OD2	5.98	123.69	118.30
1	1-C	281[A]	ARG	NE-CZ-NH2	-5.98	117.31	120.30
1	1-D	203[A]	ASP	CB-CG-OD1	5.95	123.66	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1-F	193[A]	LEU	CA-CB-CG	-5.92	101.69	115.30
1	1-C	6[A]	ASP	CB-CG-OD2	5.91	123.61	118.30
1	1-D	255[A]	ASP	CB-CG-OD2	5.88	123.59	118.30
1	1-C	193[A]	LEU	CB-CG-CD1	-5.84	101.08	111.00
1	1-C	57[A]	LEU	CB-CG-CD2	-5.83	101.08	111.00
1	1-A	2[A]	ASP	CB-CG-OD2	5.78	123.50	118.30
1	1-G	6[A]	ASP	CB-CG-OD2	5.76	123.48	118.30
1	1-I	255[A]	ASP	CB-CG-OD2	5.76	123.48	118.30
1	1-J	74[A]	ARG	NE-CZ-NH2	-5.75	117.42	120.30
1	1-I	401[A]	ASP	CB-CG-OD2	5.75	123.48	118.30
1	1-E	413[A]	ASP	CB-CG-OD2	5.75	123.47	118.30
1	1-E	219[A]	ASP	CB-CG-OD1	-5.74	113.14	118.30
1	1-B	50[A]	CYS	CA-CB-SG	5.73	124.32	114.00
1	1-B	50[B]	CYS	CA-CB-SG	5.73	124.32	114.00
1	1-F	2[A]	ASP	CB-CG-OD2	5.73	123.46	118.30
1	1-I	140[A]	ASP	CB-CG-OD2	5.71	123.44	118.30
1	1-E	219[A]	ASP	CB-CG-OD2	5.69	123.42	118.30
2	1-N	162[A]	ASP	CB-CG-OD2	5.69	123.42	118.30
1	1-B	442[A]	CYS	CA-CB-SG	-5.65	103.82	114.00
1	1-H	255[A]	ASP	CB-CG-OD1	5.64	123.37	118.30
1	1-F	15[A]	GLY	N-CA-C	-5.63	99.01	113.10
1	1-A	436[A]	LEU	CB-CG-CD1	-5.63	101.43	111.00
1	1-C	172[A]	LEU	CA-CB-CG	-5.62	102.37	115.30
1	1-A	86[A]	ASP	CB-CG-OD2	5.61	123.35	118.30
1	1-B	140[A]	ASP	CB-CG-OD2	5.61	123.35	118.30
1	1-C	199[A]	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	1-A	355[A]	PRO	N-CD-CG	-5.58	94.82	103.20
1	1-H	41[A]	LEU	CB-CG-CD2	-5.57	101.53	111.00
1	1-F	133[A]	ASP	CB-CG-OD2	5.55	123.30	118.30
1	1-J	279[A]	GLY	N-CA-C	5.55	126.98	113.10
1	1-A	280[A]	ARG	NE-CZ-NH2	5.55	123.07	120.30
1	1-I	399[A]	ASP	CB-CG-OD2	5.53	123.27	118.30
1	1-C	228[A]	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	1-D	251[A]	ASP	CB-CG-OD2	5.52	123.27	118.30
1	1-J	70[A]	ASP	CB-CG-OD2	5.50	123.25	118.30
1	1-I	50[A]	CYS	CA-CB-SG	5.48	123.87	114.00
1	1-I	50[B]	CYS	CA-CB-SG	5.48	123.87	114.00
1	1-I	6[A]	ASP	CB-CG-OD2	5.47	123.23	118.30
1	1-B	416[A]	LEU	CB-CG-CD1	-5.44	101.75	111.00
1	1-C	407[A]	LEU	CA-CB-CG	-5.42	102.84	115.30
1	1-F	272[A]	ASP	CB-CG-OD2	5.42	123.17	118.30
1	1-F	350[A]	ASP	CB-CG-OD2	5.42	123.17	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1-E	350[A]	ASP	CB-CG-OD2	5.41	123.17	118.30
1	1-J	163[A]	ASP	CB-CG-OD2	5.40	123.16	118.30
1	1-H	133[A]	ASP	CB-CG-OD2	5.40	123.16	118.30
1	1-J	203[A]	ASP	CB-CG-OD2	5.40	123.16	118.30
1	1-J	401[A]	ASP	CB-CG-OD2	5.36	123.12	118.30
1	1-F	413[A]	ASP	CB-CG-OD2	5.35	123.11	118.30
2	1-K	145[A]	ASP	CB-CG-OD2	5.33	123.10	118.30
1	1-B	15[A]	GLY	N-CA-C	-5.31	99.82	113.10
1	1-A	434[A]	LEU	CB-CG-CD2	-5.31	101.97	111.00
1	1-E	70[A]	ASP	CB-CG-OD2	5.30	123.07	118.30
2	1-M	145[A]	ASP	CB-CG-OD2	5.30	123.07	118.30
2	1-K	162[A]	ASP	CB-CG-OD2	5.29	123.06	118.30
1	1-B	320[A]	ASP	CB-CG-OD2	5.26	123.04	118.30
1	1-A	333[A]	ASP	CB-CG-OD2	5.25	123.02	118.30
1	1-F	99[A]	LEU	CB-CG-CD2	-5.25	102.08	111.00
1	1-F	320[A]	ASP	CB-CG-OD2	5.24	123.02	118.30
1	1-I	320[A]	ASP	CB-CG-OD2	5.22	123.00	118.30
1	1-H	301[A]	ARG	NE-CZ-NH1	-5.20	117.70	120.30
1	1-B	86[A]	ASP	CB-CG-OD2	5.18	122.96	118.30
1	1-C	203[A]	ASP	CB-CG-OD2	5.17	122.96	118.30
1	1-D	278[A]	ILE	CB-CA-C	-5.17	101.26	111.60
1	1-A	6[A]	ASP	CB-CG-OD2	5.17	122.95	118.30
1	1-D	44[A]	THR	OG1-CB-CG2	-5.16	98.12	110.00
1	1-E	6[A]	ASP	CB-CG-OD2	5.13	122.92	118.30
1	1-F	16[A]	PRO	C-N-CA	-5.08	111.63	122.30
1	1-A	163[A]	ASP	CB-CG-OD2	5.07	122.86	118.30
1	1-C	8[A]	ASP	CB-CG-OD2	5.04	122.83	118.30
1	1-E	326[A]	MET	CG-SD-CE	5.00	108.21	100.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	1-L	136[A]	ARG	Sidechain
2	2-K	136[C]	ARG	Sidechain

## 4.2 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	1-A	3521	0	3577	185	0
1	1-B	3521	0	3577	189	0
1	1-C	3521	0	3577	189	0
1	1-D	3521	0	3577	203	0
1	1-E	3521	0	3577	191	0
1	1-F	3521	0	3577	180	0
1	1-G	3521	0	3577	208	0
1	1-H	3521	0	3577	188	0
1	1-I	3521	0	3577	255	0
1	1-J	3521	0	3577	217	0
1	2-A	3521	0	3577	183	0
1	2-B	3521	0	3577	190	0
1	2-C	3521	0	3577	190	0
1	2-D	3521	0	3577	210	0
1	2-E	3521	0	3577	195	0
1	2-F	3521	0	3577	172	0
1	2-G	3521	0	3577	211	0
1	2-H	3521	0	3577	192	0
1	2-I	3521	0	3577	255	0
1	2-J	3521	0	3577	211	0
2	1-K	331	0	347	65	0
2	1-L	331	0	346	54	0
2	1-M	331	0	347	80	0
2	1-N	331	0	347	57	0
2	1-O	331	0	347	33	0
2	2-K	320	0	337	39	0
2	2-L	320	0	337	46	0
2	2-M	327	0	344	51	0
2	2-N	320	0	337	58	0
3	1-A	53	0	31	8	0
3	1-B	53	0	31	11	0
3	1-C	53	0	31	8	0
3	1-D	53	0	31	5	0
3	1-E	53	0	31	4	0
3	1-F	53	0	31	10	0
3	1-G	53	0	30	2	0
3	1-H	53	0	31	4	0
3	1-I	53	0	31	11	0
3	1-J	53	0	0	0	0
3	2-A	53	0	31	11	0
3	2-B	53	0	31	7	0
3	2-C	53	0	31	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	2-D	53	0	31	4	0
3	2-E	53	0	31	10	0
3	2-F	53	0	30	2	0
3	2-G	53	0	31	4	0
3	2-H	53	0	31	9	0
3	2-I	53	0	31	17	0
3	2-O	53	0	31	8	0
4	1-A	39	0	0	5	0
4	1-B	50	0	0	2	0
4	1-C	76	0	0	9	0
4	1-D	63	0	0	6	0
4	1-E	68	0	0	5	0
4	1-F	42	0	0	9	0
4	1-G	35	0	0	1	0
4	1-H	67	0	0	11	0
4	1-I	18	0	0	6	0
4	1-J	30	0	31	21	0
4	1-M	2	0	0	0	0
4	1-O	2	0	0	0	0
4	2-A	50	0	0	2	0
4	2-B	76	0	0	10	0
4	2-C	63	0	0	6	0
4	2-D	67	0	0	5	0
4	2-E	42	0	0	9	0
4	2-F	34	0	0	1	0
4	2-G	66	0	0	11	0
4	2-H	19	0	0	8	0
4	2-I	31	0	0	4	0
4	2-J	42	0	0	5	0
4	2-M	2	0	0	0	0
All	All	75406	0	75247	4261	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 29.

All (4261) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:172[C]:THR:CB	2:M:172[C]:THR:CG2	1.77	1.61
1:E:220[A]:MET:CE	1:E:220[A]:MET:SD	2.01	1.48
1:E:220[C]:MET:SD	1:E:220[C]:MET:CE	2.01	1.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:65[A]:MET:CE	1:C:65[A]:MET:SD	2.02	1.47
1:C:65[C]:MET:CE	1:C:65[C]:MET:SD	2.02	1.47
1:D:65[A]:MET:CE	1:D:65[A]:MET:SD	2.04	1.46
1:D:65[C]:MET:CE	1:D:65[C]:MET:SD	2.04	1.46
1:G:65[A]:MET:CE	1:G:65[A]:MET:SD	2.03	1.45
1:G:65[C]:MET:CE	1:G:65[C]:MET:SD	2.03	1.45
1:D:220[A]:MET:CE	1:D:220[A]:MET:SD	2.03	1.45
1:D:220[C]:MET:CE	1:D:220[C]:MET:SD	2.03	1.45
1:B:326[A]:MET:CE	1:B:326[A]:MET:SD	2.04	1.44
1:B:326[C]:MET:CE	1:B:326[C]:MET:SD	2.04	1.44
1:B:65[A]:MET:CE	1:B:65[A]:MET:SD	2.08	1.41
1:B:65[C]:MET:CE	1:B:65[C]:MET:SD	2.08	1.41
1:F:403[A]:MET:CE	1:F:403[A]:MET:SD	2.09	1.40
1:F:403[C]:MET:SD	1:F:403[C]:MET:CE	2.09	1.40
1:C:326[A]:MET:SD	1:C:326[A]:MET:CE	2.08	1.40
1:C:326[C]:MET:CE	1:C:326[C]:MET:SD	2.08	1.40
1:H:220[A]:MET:CE	1:H:220[A]:MET:SD	2.10	1.40
1:H:220[C]:MET:CE	1:H:220[C]:MET:SD	2.10	1.40
1:D:326[A]:MET:CE	1:D:326[A]:MET:SD	2.11	1.39
1:D:326[C]:MET:CE	1:D:326[C]:MET:SD	2.11	1.39
1:C:220[A]:MET:CE	1:C:220[A]:MET:SD	2.14	1.35
1:C:220[C]:MET:CE	1:C:220[C]:MET:SD	2.14	1.35
1:I:305[A]:ASN:HB3	4:I:4763[A]:HOH:O	1.30	1.30
4:H:4763[C]:HOH:O	1:I:305[C]:ASN:HB3	1.30	1.30
1:A:220[A]:MET:CE	1:A:220[A]:MET:SD	2.23	1.27
1:A:220[C]:MET:CE	1:A:220[C]:MET:SD	2.23	1.27
1:E:255[A]:ASP:OD1	1:E:270[A]:THR:HB	1.38	1.22
1:E:255[C]:ASP:OD1	1:E:270[C]:THR:HB	1.38	1.22
1:G:348[C]:HIS:CE1	2:N:136[C]:ARG:HD2	1.78	1.17
1:D:69[A]:LYS:HB3	4:D:4792[A]:HOH:O	1.44	1.16
4:C:4792[C]:HOH:O	1:D:69[C]:LYS:HB3	1.44	1.16
1:G:445[A]:ILE:HD13	1:G:445[A]:ILE:O	1.46	1.15
1:G:445[C]:ILE:O	1:G:445[C]:ILE:HD13	1.46	1.15
1:F:348[A]:HIS:CD2	2:M:136[A]:ARG:HH11	1.66	1.14
1:B:3[A]:GLN:HG2	1:B:4[A]:PRO:HD2	1.29	1.13
1:B:3[C]:GLN:HG2	1:B:4[C]:PRO:HD2	1.29	1.13
2:N:168[A]:GLN:HA	2:N:168[A]:GLN:NE2	1.52	1.12
1:F:345[A]:GLY:HA2	2:M:141[A]:LYS:HD3	1.31	1.10
1:H:46[A]:LEU:HD21	1:H:100[A]:THR:HG22	1.33	1.10
1:H:46[C]:LEU:HD21	1:H:100[C]:THR:HG22	1.33	1.10
1:G:348[C]:HIS:HE1	2:N:136[C]:ARG:HD2	0.98	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:170[C]:LYS:O	2:N:171[C]:GLN:HB2	1.47	1.10
1:J:346[A]:ALA:HB1	2:O:140[A]:GLU:OE1	1.52	1.09
2:K:152[A]:THR:HG22	2:K:153[A]:GLY:H	1.17	1.09
1:D:406[A]:ILE:HD11	1:D:463[A]:ASN:HA	1.11	1.09
1:D:406[C]:ILE:HD11	1:D:463[C]:ASN:HA	1.11	1.09
1:G:445[A]:ILE:HD13	1:G:445[A]:ILE:C	1.73	1.08
1:G:445[C]:ILE:HD13	1:G:445[C]:ILE:C	1.73	1.08
2:M:145[C]:ASP:O	2:M:148[C]:GLN:HG2	1.55	1.06
2:N:168[C]:GLN:HE21	2:N:168[C]:GLN:HA	0.94	1.06
2:M:159[A]:THR:HG22	2:M:161[A]:GLU:H	1.08	1.06
1:C:74[A]:ARG:HD3	1:D:59[A]:ASN:OD1	1.56	1.06
1:C:74[C]:ARG:HD3	1:D:59[C]:ASN:OD1	1.56	1.06
1:I:11[A]:VAL:HG13	1:I:145[A]:LEU:HD23	1.37	1.05
1:I:11[C]:VAL:HG13	1:I:145[C]:LEU:HD23	1.37	1.05
1:H:124[A]:LYS:HD3	1:H:124[A]:LYS:H	1.21	1.05
1:H:124[C]:LYS:H	1:H:124[C]:LYS:HD3	1.21	1.05
1:I:218[A]:ILE:H	1:I:218[A]:ILE:HD13	1.18	1.05
1:I:218[C]:ILE:HD13	1:I:218[C]:ILE:H	1.18	1.05
1:G:339[A]:VAL:HG12	1:G:342[A]:MET:HE3	1.38	1.05
1:G:339[C]:VAL:HG12	1:G:342[C]:MET:HE3	1.38	1.05
2:N:160[C]:LYS:HE3	2:N:164[C]:LEU:HD11	1.38	1.04
2:M:131[A]:LEU:HD13	2:M:136[A]:ARG:HE	0.93	1.04
1:A:1[A]:ALA:HB2	1:A:136[A]:THR:HG23	1.39	1.04
2:M:159[A]:THR:HG22	2:M:161[A]:GLU:N	1.71	1.04
1:A:1[C]:ALA:HB2	1:A:136[C]:THR:HG23	1.39	1.04
1:I:409[A]:GLN:HG2	1:I:412[A]:THR:OG1	1.58	1.03
2:L:144[A]:LEU:HD11	2:L:166[A]:LEU:HB3	1.39	1.03
1:I:409[C]:GLN:HG2	1:I:412[C]:THR:OG1	1.58	1.03
1:F:312[A]:ILE:HG12	1:F:315[A]:ILE:HG13	1.40	1.03
1:F:312[C]:ILE:HG12	1:F:315[C]:ILE:HG13	1.40	1.03
1:F:44[A]:THR:CG2	3:F:4755[A]:FAD:O2A	2.07	1.02
3:E:4755[C]:FAD:O2A	1:F:44[C]:THR:CG2	2.07	1.02
2:M:159[C]:THR:HG22	2:M:162[C]:ASP:H	1.21	1.02
1:E:409[A]:GLN:NE2	1:E:411[A]:SER:H	1.56	1.02
1:E:409[C]:GLN:NE2	1:E:411[C]:SER:H	1.56	1.02
2:N:133[A]:PRO:HA	2:N:136[A]:ARG:HE	1.21	1.02
2:N:168[A]:GLN:HE21	2:N:168[A]:GLN:CA	1.72	1.02
2:M:131[A]:LEU:HD13	2:M:136[A]:ARG:NE	1.74	1.02
1:F:44[A]:THR:HG23	3:F:4755[A]:FAD:PA	2.01	1.00
1:J:51[A]:ILE:HB	1:J:52[A]:PRO:HD3	1.42	1.00
3:E:4755[C]:FAD:PA	1:F:44[C]:THR:HG23	2.01	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:51[C]:ILE:HB	1:J:52[C]:PRO:HD3	1.42	1.00
1:I:110[A]:ASN:HD22	1:I:110[A]:ASN:N	1.57	1.00
1:I:110[C]:ASN:HD22	1:I:110[C]:ASN:N	1.57	1.00
2:N:159[C]:THR:CG2	2:N:161[C]:GLU:HB2	1.91	1.00
2:N:136[A]:ARG:HG3	2:N:137[A]:ASN:N	1.74	1.00
1:I:448[A]:VAL:HG21	1:J:434[A]:LEU:HD13	1.39	0.99
1:I:448[C]:VAL:HG21	1:J:434[C]:LEU:HD13	1.39	0.99
1:C:78[A]:MET:HE2	1:D:81[A]:VAL:HG22	1.45	0.99
1:C:78[C]:MET:HE2	1:D:81[C]:VAL:HG22	1.45	0.99
1:G:96[A]:VAL:HG12	1:G:97[A]:LYS:HD3	1.44	0.99
1:G:96[C]:VAL:HG12	1:G:97[C]:LYS:HD3	1.44	0.99
1:A:44[A]:THR:HG23	3:A:4750[A]:FAD:PA	2.02	0.99
1:A:44[C]:THR:HG23	3:O:4750[C]:FAD:PA	2.02	0.99
2:N:168[C]:GLN:HA	2:N:168[C]:GLN:NE2	1.78	0.99
1:G:358[A]:ILE:HD11	1:G:360[A]:THR:HG23	1.42	0.98
1:J:289[A]:LEU:HD22	1:J:294[A]:ILE:HD12	1.46	0.98
1:G:358[C]:ILE:HD11	1:G:360[C]:THR:HG23	1.42	0.98
1:J:289[C]:LEU:HD22	1:J:294[C]:ILE:HD12	1.46	0.98
1:I:41[A]:LEU:H	1:I:41[A]:LEU:HD12	1.27	0.98
1:I:41[C]:LEU:H	1:I:41[C]:LEU:HD12	1.27	0.98
1:J:345[A]:GLY:HA2	2:O:141[A]:LYS:HD2	1.45	0.96
1:A:44[A]:THR:HG23	3:A:4750[A]:FAD:O2A	1.63	0.96
1:E:447[A]:ARG:HG2	1:E:447[A]:ARG:HH11	1.29	0.96
1:A:44[C]:THR:HG23	3:O:4750[C]:FAD:O2A	1.63	0.96
1:E:447[C]:ARG:HG2	1:E:447[C]:ARG:HH11	1.29	0.96
2:K:159[A]:THR:HG22	2:K:161[A]:GLU:N	1.81	0.96
2:K:159[A]:THR:HG22	2:K:161[A]:GLU:H	1.30	0.96
2:M:131[A]:LEU:CD1	2:M:136[A]:ARG:HE	1.77	0.96
1:F:348[A]:HIS:HD2	2:M:136[A]:ARG:HH11	0.98	0.95
1:D:69[A]:LYS:CB	4:D:4792[A]:HOH:O	2.06	0.95
4:C:4792[C]:HOH:O	1:D:69[C]:LYS:CB	2.06	0.95
2:N:131[C]:LEU:HD21	2:N:146[C]:ALA:CB	1.96	0.95
1:C:414[A]:ARG:HH11	1:C:414[A]:ARG:CG	1.80	0.94
1:C:414[C]:ARG:CG	1:C:414[C]:ARG:HH11	1.80	0.94
2:M:159[C]:THR:HG22	2:M:162[C]:ASP:N	1.81	0.94
1:E:80[A]:GLU:H	1:F:79[A]:SER:HB2	1.33	0.94
1:E:80[C]:GLU:H	1:F:79[C]:SER:HB2	1.33	0.94
2:L:134[C]:ALA:O	2:L:138[C]:ILE:HG22	1.67	0.93
1:E:169[A]:THR:HG22	4:E:4759[A]:HOH:O	1.68	0.93
4:D:4759[C]:HOH:O	1:E:169[C]:THR:HG22	1.68	0.93
1:E:188[A]:VAL:HG22	1:E:358[A]:ILE:CD1	1.99	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:188[C]:VAL:HG22	1:E:358[C]:ILE:CD1	1.99	0.93
1:G:358[A]:ILE:HG23	1:G:364[A]:VAL:HB	1.49	0.92
1:J:406[A]:ILE:HD13	1:J:406[A]:ILE:H	1.33	0.92
2:N:141[A]:LYS:O	2:N:142[A]:HIS:HD2	1.51	0.92
1:G:358[C]:ILE:HG23	1:G:364[C]:VAL:HB	1.49	0.92
1:J:406[C]:ILE:HD13	1:J:406[C]:ILE:H	1.33	0.92
2:K:136[C]:ARG:HG2	2:K:136[C]:ARG:O	1.66	0.92
2:N:130[A]:ARG:N	2:N:157[A]:ILE:HG22	1.84	0.92
1:G:339[A]:VAL:HG12	1:G:342[A]:MET:CE	1.98	0.92
1:G:339[C]:VAL:HG12	1:G:342[C]:MET:CE	1.98	0.92
1:I:218[A]:ILE:HD13	1:I:218[A]:ILE:N	1.81	0.92
1:I:218[C]:ILE:HD13	1:I:218[C]:ILE:N	1.81	0.92
1:D:409[A]:GLN:HE21	1:D:411[A]:SER:H	1.08	0.92
2:K:152[A]:THR:HG22	2:K:153[A]:GLY:N	1.84	0.92
1:D:409[C]:GLN:HE21	1:D:411[C]:SER:H	1.08	0.92
1:F:44[A]:THR:HG23	3:F:4755[A]:FAD:O2A	1.67	0.92
3:E:4755[C]:FAD:O2A	1:F:44[C]:THR:HG23	1.67	0.92
1:D:51[A]:ILE:HB	1:D:52[A]:PRO:HD3	1.51	0.92
1:D:51[C]:ILE:HB	1:D:52[C]:PRO:HD3	1.51	0.92
2:N:168[C]:GLN:HE21	2:N:168[C]:GLN:CA	1.79	0.91
1:G:57[A]:LEU:HD11	1:G:192[A]:GLU:HG2	1.52	0.91
1:J:406[A]:ILE:HD12	1:J:462[A]:ALA:HB1	1.52	0.91
1:G:57[C]:LEU:HD11	1:G:192[C]:GLU:HG2	1.52	0.91
1:J:406[C]:ILE:HD12	1:J:462[C]:ALA:HB1	1.52	0.91
1:D:406[A]:ILE:CD1	1:D:463[A]:ASN:HA	1.99	0.91
1:F:124[A]:LYS:HG2	1:F:312[A]:ILE:CD1	2.01	0.91
1:D:406[C]:ILE:CD1	1:D:463[C]:ASN:HA	1.99	0.91
1:F:124[C]:LYS:HG2	1:F:312[C]:ILE:CD1	2.01	0.91
1:D:406[A]:ILE:HD11	1:D:463[A]:ASN:CA	1.99	0.91
1:D:406[C]:ILE:HD11	1:D:463[C]:ASN:CA	1.99	0.91
1:J:345[A]:GLY:HA2	2:O:141[A]:LYS:CD	2.01	0.91
2:N:141[A]:LYS:O	2:N:142[A]:HIS:CD2	2.24	0.90
2:K:130[A]:ARG:HG2	2:K:130[A]:ARG:HH11	1.36	0.90
1:I:266[A]:ALA:O	1:I:267[A]:GLU:HB2	1.66	0.90
1:I:266[C]:ALA:O	1:I:267[C]:GLU:HB2	1.66	0.90
1:B:46[A]:LEU:HD12	1:B:46[A]:LEU:O	1.72	0.90
1:B:46[C]:LEU:HD12	1:B:46[C]:LEU:O	1.72	0.90
1:G:442[A]:CYS:HA	1:G:463[A]:ASN:HD22	1.36	0.90
1:G:442[C]:CYS:HA	1:G:463[C]:ASN:HD22	1.36	0.90
1:H:127[A]:VAL:HG21	1:H:144[A]:ILE:HD12	1.51	0.90
1:H:127[C]:VAL:HG21	1:H:144[C]:ILE:HD12	1.51	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:177[A]:VAL:HG11	1:G:200[A]:LEU:HB3	1.54	0.89
1:G:177[C]:VAL:HG11	1:G:200[C]:LEU:HB3	1.54	0.89
2:N:136[A]:ARG:HG3	2:N:137[A]:ASN:H	1.32	0.89
1:F:42[A]:GLY:HA3	1:F:46[A]:LEU:HD23	1.54	0.89
1:F:42[C]:GLY:HA3	1:F:46[C]:LEU:HD23	1.54	0.89
1:G:137[A]:GLN:HE21	1:G:138[A]:VAL:H	1.17	0.89
2:N:168[A]:GLN:HA	2:N:168[A]:GLN:HE21	0.77	0.89
1:G:137[C]:GLN:HE21	1:G:138[C]:VAL:H	1.17	0.89
1:C:3[A]:GLN:HG3	1:C:4[A]:PRO:HD2	1.54	0.89
1:I:372[A]:GLU:O	1:I:374[A]:LEU:N	2.06	0.89
1:J:67[A]:HIS:HA	1:J:81[A]:VAL:HG11	1.55	0.89
1:C:3[C]:GLN:HG3	1:C:4[C]:PRO:HD2	1.54	0.89
1:I:372[C]:GLU:O	1:I:374[C]:LEU:N	2.06	0.89
1:J:67[C]:HIS:HA	1:J:81[C]:VAL:HG11	1.55	0.89
2:N:153[C]:GLY:O	2:N:154[C]:PRO:O	1.91	0.89
1:I:358[A]:ILE:HG23	1:I:364[A]:VAL:HB	1.53	0.88
1:I:358[C]:ILE:HG23	1:I:364[C]:VAL:HB	1.53	0.88
2:M:150[A]:THR:CG2	2:M:151[A]:ALA:N	2.36	0.88
1:C:51[A]:ILE:HB	1:C:52[A]:PRO:HD3	1.56	0.88
1:C:51[C]:ILE:HB	1:C:52[C]:PRO:HD3	1.56	0.88
1:E:312[A]:ILE:HD13	1:E:312[A]:ILE:C	1.92	0.88
1:E:312[C]:ILE:HD13	1:E:312[C]:ILE:C	1.92	0.88
1:G:409[A]:GLN:HE21	1:G:411[A]:SER:H	1.19	0.88
1:G:409[C]:GLN:HE21	1:G:411[C]:SER:H	1.19	0.88
2:M:159[C]:THR:HG23	2:M:161[C]:GLU:H	1.39	0.88
1:I:319[A]:GLY:HA3	3:I:4759[A]:HOH:O	1.73	0.87
4:H:4759[C]:HOH:O	1:I:319[C]:GLY:HA3	1.73	0.87
1:A:46[A]:LEU:O	1:A:46[A]:LEU:HD12	1.73	0.87
2:N:133[A]:PRO:HA	2:N:136[A]:ARG:NE	1.90	0.87
1:A:46[C]:LEU:HD12	1:A:46[C]:LEU:O	1.73	0.87
1:F:392[A]:SER:HB2	4:F:4793[A]:HOH:O	1.74	0.87
1:I:14[A]:SER:HB3	1:I:42[A]:GLY:H	1.39	0.87
1:I:249[A]:LYS:HD3	1:I:255[A]:ASP:OD2	1.75	0.87
1:I:448[A]:VAL:HG21	1:J:434[A]:LEU:CD1	2.03	0.87
2:L:151[A]:ALA:CB	2:L:158[A]:PHE:HA	2.05	0.87
4:E:4793[C]:HOH:O	1:F:392[C]:SER:HB2	1.74	0.87
1:I:14[C]:SER:HB3	1:I:42[C]:GLY:H	1.39	0.87
1:I:249[C]:LYS:HD3	1:I:255[C]:ASP:OD2	1.75	0.87
1:I:448[C]:VAL:HG21	1:J:434[C]:LEU:CD1	2.03	0.87
2:L:148[C]:GLN:HB2	2:L:166[C]:LEU:HD11	1.56	0.87
1:D:162[A]:GLU:OE1	1:D:162[A]:GLU:HA	1.75	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:162[C]:GLU:OE1	1:D:162[C]:GLU:HA	1.75	0.86
1:A:358[A]:ILE:CD1	1:A:360[A]:THR:HG23	2.05	0.86
1:A:358[C]:ILE:CD1	1:A:360[C]:THR:HG23	2.05	0.86
1:D:44[A]:THR:HG23	3:D:4753[A]:FAD:O2A	1.75	0.86
1:G:54[A]:LYS:HE2	1:G:359[A]:TYR:CD2	2.10	0.86
1:G:314[A]:ASN:H	1:G:314[A]:ASN:HD22	1.21	0.86
3:C:4753[C]:FAD:O2A	1:D:44[C]:THR:HG23	1.75	0.86
1:G:54[C]:LYS:HE2	1:G:359[C]:TYR:CD2	2.10	0.86
1:G:314[C]:ASN:H	1:G:314[C]:ASN:HD22	1.21	0.86
1:I:297[A]:ASP:OD2	1:I:301[A]:ARG:HG3	1.74	0.86
1:I:297[C]:ASP:OD2	1:I:301[C]:ARG:HG3	1.74	0.86
2:K:131[A]:LEU:HD23	2:K:136[A]:ARG:CB	2.06	0.86
1:H:127[A]:VAL:CG2	1:H:144[A]:ILE:HD12	2.04	0.85
1:H:127[C]:VAL:CG2	1:H:144[C]:ILE:HD12	2.04	0.85
2:M:150[A]:THR:HG23	2:M:151[A]:ALA:H	1.38	0.85
2:N:160[C]:LYS:CE	2:N:164[C]:LEU:HD11	2.05	0.85
1:A:44[A]:THR:CG2	3:A:4750[A]:FAD:O2A	2.24	0.85
1:A:44[C]:THR:CG2	3:O:4750[C]:FAD:O2A	2.24	0.85
2:N:131[C]:LEU:HD21	2:N:146[C]:ALA:HB2	1.55	0.85
1:C:444[C]:ASP:OD1	2:L:155[C]:ARG:HD3	1.75	0.85
1:B:137[A]:GLN:HE21	1:B:137[A]:GLN:C	1.78	0.85
1:G:358[A]:ILE:HD11	1:G:360[A]:THR:CG2	2.06	0.85
2:K:144[A]:LEU:HD13	2:K:166[A]:LEU:HD23	1.58	0.85
1:B:137[C]:GLN:HE21	1:B:137[C]:GLN:C	1.78	0.85
1:G:358[C]:ILE:HD11	1:G:360[C]:THR:CG2	2.06	0.85
1:D:330[A]:LYS:HE2	1:D:334[A]:GLU:OE2	1.76	0.85
1:D:330[C]:LYS:HE2	1:D:334[C]:GLU:OE2	1.76	0.85
1:G:472[A]:ILE:C	1:G:472[A]:ILE:HD13	1.97	0.85
2:K:136[A]:ARG:HA	2:K:139[A]:LEU:HD12	1.59	0.85
1:G:472[C]:ILE:C	1:G:472[C]:ILE:HD13	1.97	0.85
1:H:19[A]:TYR:O	1:H:23[A]:ILE:HG13	1.76	0.85
1:H:42[A]:GLY:HA3	1:H:46[A]:LEU:HD23	1.59	0.85
1:H:19[C]:TYR:O	1:H:23[C]:ILE:HG13	1.76	0.85
1:H:42[C]:GLY:HA3	1:H:46[C]:LEU:HD23	1.59	0.85
1:G:445[A]:ILE:C	1:G:445[A]:ILE:CD1	2.45	0.84
1:G:445[C]:ILE:C	1:G:445[C]:ILE:CD1	2.45	0.84
1:A:45[A]:CYS:HG	1:A:50[A]:CYS:CB	1.88	0.84
1:A:45[C]:CYS:HG	1:A:50[C]:CYS:CB	1.88	0.84
1:C:250[A]:SER:HB3	1:E:304[A]:VAL:HG23	1.57	0.84
1:C:250[C]:SER:HB3	1:E:304[C]:VAL:HG23	1.57	0.84
1:F:45[A]:CYS:HG	1:F:50[A]:CYS:HG	1.05	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:44[A]:THR:HG23	3:G:4756[A]:FAD:O2A	1.77	0.84
1:F:45[C]:CYS:HG	1:F:50[C]:CYS:HG	1.05	0.84
3:F:4756[C]:FAD:O2A	1:G:44[C]:THR:HG23	1.77	0.84
1:C:430[A]:ASN:HD22	1:D:456[A]:SER:CB	1.89	0.84
1:C:430[C]:ASN:HD22	1:D:456[C]:SER:CB	1.89	0.84
2:N:141[A]:LYS:O	2:N:141[A]:LYS:CG	2.26	0.84
1:F:144[A]:ILE:HD11	1:F:146[A]:ILE:HD13	1.58	0.83
1:G:110[A]:ASN:O	1:G:111[A]:LYS:HG3	1.77	0.83
1:F:144[C]:ILE:HD11	1:F:146[C]:ILE:HD13	1.58	0.83
1:G:110[C]:ASN:O	1:G:111[C]:LYS:HG3	1.77	0.83
1:C:137[A]:GLN:HE21	1:C:137[A]:GLN:C	1.81	0.83
1:C:137[C]:GLN:C	1:C:137[C]:GLN:HE21	1.81	0.83
1:E:137[A]:GLN:HE21	1:E:137[A]:GLN:CA	1.87	0.83
1:F:348[A]:HIS:CD2	2:M:136[A]:ARG:NH1	2.46	0.83
1:J:305[A]:ASN:HD21	1:J:309[A]:GLN:CG	1.91	0.83
1:E:137[C]:GLN:HE21	1:E:137[C]:GLN:CA	1.87	0.83
1:J:305[C]:ASN:HD21	1:J:309[C]:GLN:CG	1.91	0.83
2:L:151[A]:ALA:HB1	2:L:162[A]:ASP:OD2	1.79	0.83
1:E:409[A]:GLN:HE21	1:E:411[A]:SER:H	1.21	0.83
1:E:409[C]:GLN:HE21	1:E:411[C]:SER:H	1.21	0.83
1:B:137[A]:GLN:HE21	1:B:137[A]:GLN:CA	1.92	0.83
1:B:137[C]:GLN:HE21	1:B:137[C]:GLN:CA	1.92	0.83
2:N:159[C]:THR:HG22	2:N:161[C]:GLU:HB2	1.58	0.83
1:H:150[A]:SER:OG	1:H:280[A]:ARG:NH1	2.11	0.83
1:H:150[C]:SER:OG	1:H:280[C]:ARG:NH1	2.11	0.83
1:F:348[A]:HIS:HD2	2:M:136[A]:ARG:NH1	1.77	0.83
1:B:45[A]:CYS:HG	1:B:50[A]:CYS:HG	0.84	0.83
1:B:45[C]:CYS:HG	1:B:50[C]:CYS:HG	0.84	0.83
2:K:130[C]:ARG:O	2:K:157[C]:ILE:HG23	1.79	0.82
1:G:169[A]:THR:HB	4:G:4760[A]:HOH:O	1.79	0.82
2:N:141[A]:LYS:O	2:N:141[A]:LYS:HG2	1.78	0.82
4:F:4760[C]:HOH:O	1:G:169[C]:THR:HB	1.79	0.82
2:L:132[A]:SER:O	2:L:134[A]:ALA:N	2.12	0.82
1:H:305[A]:ASN:C	1:H:305[A]:ASN:HD22	1.80	0.82
1:J:406[A]:ILE:HD13	1:J:406[A]:ILE:N	1.93	0.82
1:H:305[C]:ASN:C	1:H:305[C]:ASN:HD22	1.80	0.82
1:J:406[C]:ILE:HD13	1:J:406[C]:ILE:N	1.93	0.82
1:H:222[A]:ILE:HD11	4:H:4775[A]:HOH:O	1.79	0.82
4:G:4775[C]:HOH:O	1:H:222[C]:ILE:HD11	1.79	0.82
2:N:131[A]:LEU:HD23	2:N:136[A]:ARG:HA	1.62	0.82
1:A:188[A]:VAL:HG23	1:A:189[A]:ILE:HD12	1.60	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:220[A]:MET:CE	1:H:220[A]:MET:HB3	2.10	0.82
1:A:188[C]:VAL:HG23	1:A:189[C]:ILE:HD12	1.60	0.82
1:H:220[C]:MET:CE	1:H:220[C]:MET:HB3	2.10	0.82
1:I:319[A]:GLY:O	1:I:330[A]:LYS:NZ	2.12	0.82
1:I:319[C]:GLY:O	1:I:330[C]:LYS:NZ	2.12	0.82
2:M:159[C]:THR:HG23	2:M:161[C]:GLU:N	1.94	0.82
2:K:131[A]:LEU:HD23	2:K:136[A]:ARG:HB3	1.60	0.81
1:B:137[A]:GLN:HE21	1:B:138[A]:VAL:N	1.77	0.81
1:B:137[C]:GLN:HE21	1:B:138[C]:VAL:N	1.77	0.81
1:B:51[A]:ILE:HB	1:B:52[A]:PRO:HD3	1.61	0.81
1:C:430[A]:ASN:ND2	1:D:456[A]:SER:HB2	1.96	0.81
1:J:305[A]:ASN:HD21	1:J:309[A]:GLN:HG2	1.44	0.81
1:B:51[C]:ILE:HB	1:B:52[C]:PRO:HD3	1.61	0.81
1:C:430[C]:ASN:ND2	1:D:456[C]:SER:HB2	1.96	0.81
1:J:305[C]:ASN:HD21	1:J:309[C]:GLN:HG2	1.44	0.81
1:A:79[A]:SER:HB3	1:B:79[A]:SER:HB3	1.61	0.81
1:A:79[C]:SER:HB3	1:B:79[C]:SER:HB3	1.61	0.81
1:D:193[A]:LEU:HD12	1:D:193[A]:LEU:N	1.96	0.81
1:J:406[A]:ILE:CD1	1:J:462[A]:ALA:HB1	2.11	0.81
1:D:193[C]:LEU:HD12	1:D:193[C]:LEU:N	1.96	0.81
1:J:406[C]:ILE:CD1	1:J:462[C]:ALA:HB1	2.11	0.81
1:E:366[A]:TRP:HB2	1:E:419[A]:HIS:CD2	2.16	0.81
1:E:366[C]:TRP:HB2	1:E:419[C]:HIS:CD2	2.16	0.81
1:D:188[A]:VAL:HG22	1:D:358[A]:ILE:HG12	1.62	0.81
1:D:188[C]:VAL:HG22	1:D:358[C]:ILE:HG12	1.62	0.81
2:N:170[C]:LYS:O	2:N:171[C]:GLN:CB	2.29	0.81
1:C:3[A]:GLN:HA	1:C:3[A]:GLN:HE21	1.46	0.81
1:J:188[A]:VAL:HG22	1:J:358[A]:ILE:HG12	1.61	0.81
1:C:3[C]:GLN:HE21	1:C:3[C]:GLN:HA	1.46	0.81
1:J:188[C]:VAL:HG22	1:J:358[C]:ILE:HG12	1.61	0.81
2:O:149[A]:GLY:H	2:O:166[A]:LEU:HD11	1.45	0.81
1:C:9[A]:VAL:CG2	1:C:342[A]:MET:HE1	2.11	0.80
1:I:110[A]:ASN:HD22	1:I:110[A]:ASN:H	1.27	0.80
1:C:9[C]:VAL:CG2	1:C:342[C]:MET:HE1	2.11	0.80
1:I:110[C]:ASN:HD22	1:I:110[C]:ASN:H	1.27	0.80
1:B:431[A]:GLU:OE2	1:B:450[A]:HIS:HE1	1.63	0.80
1:B:431[C]:GLU:OE2	1:B:450[C]:HIS:HE1	1.63	0.80
1:C:1[A]:ALA:O	1:C:3[A]:GLN:N	2.14	0.80
1:E:255[A]:ASP:OD1	1:E:270[A]:THR:CB	2.26	0.80
1:C:1[C]:ALA:O	1:C:3[C]:GLN:N	2.14	0.80
1:E:255[C]:ASP:OD1	1:E:270[C]:THR:CB	2.26	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:158[C]:PHE:HE2	2:N:163[C]:ALA:HA	1.47	0.80
1:A:409[A]:GLN:HE21	1:A:411[A]:SER:H	1.30	0.80
4:D:4784[A]:HOH:O	1:G:375[A]:LYS:HE2	1.81	0.80
1:G:227[A]:GLN:O	1:G:231[A]:GLN:HG3	1.82	0.80
1:A:409[C]:GLN:HE21	1:A:411[C]:SER:H	1.30	0.80
4:C:4784[C]:HOH:O	1:G:375[C]:LYS:HE2	1.81	0.80
1:G:227[C]:GLN:O	1:G:231[C]:GLN:HG3	1.82	0.80
1:B:291[A]:GLU:CD	1:B:291[A]:GLU:H	1.84	0.80
1:B:406[A]:ILE:C	1:B:406[A]:ILE:HD12	2.02	0.80
1:B:291[C]:GLU:CD	1:B:291[C]:GLU:H	1.84	0.80
1:B:406[C]:ILE:C	1:B:406[C]:ILE:HD12	2.02	0.80
1:J:468[A]:PHE:HD2	1:J:470[A]:LYS:HZ1	1.28	0.80
1:J:468[C]:PHE:HD2	1:J:470[C]:LYS:HZ1	1.28	0.80
1:C:219[A]:ASP:OD2	1:C:405[A]:LYS:NZ	2.15	0.80
1:D:307[A]:ARG:O	1:D:308[A]:PHE:HB2	1.80	0.80
1:F:124[A]:LYS:HG2	1:F:312[A]:ILE:HD12	1.64	0.80
2:L:139[A]:LEU:O	2:L:141[A]:LYS:N	2.15	0.80
1:C:219[C]:ASP:OD2	1:C:405[C]:LYS:NZ	2.15	0.80
1:D:307[C]:ARG:O	1:D:308[C]:PHE:HB2	1.80	0.80
1:F:124[C]:LYS:HG2	1:F:312[C]:ILE:HD12	1.64	0.80
2:N:148[C]:GLN:O	2:N:149[C]:GLY:O	1.99	0.79
2:M:159[A]:THR:CG2	2:M:161[A]:GLU:H	1.92	0.79
1:G:358[A]:ILE:HD13	1:G:358[A]:ILE:C	2.02	0.79
1:J:20[A]:VAL:HG11	1:J:332[A]:GLU:HG3	1.63	0.79
1:G:358[C]:ILE:C	1:G:358[C]:ILE:HD13	2.02	0.79
1:J:20[C]:VAL:HG11	1:J:332[C]:GLU:HG3	1.63	0.79
1:B:428[A]:MET:HE1	1:B:459[A]:PHE:HB2	1.64	0.79
1:H:10[A]:THR:HG23	1:H:141[A]:THR:OG1	1.83	0.79
1:B:428[C]:MET:HE1	1:B:459[C]:PHE:HB2	1.64	0.79
1:H:10[C]:THR:HG23	1:H:141[C]:THR:OG1	1.83	0.79
1:B:392[A]:SER:O	1:B:396[A]:THR:HG22	1.83	0.79
1:J:330[A]:LYS:HE2	1:J:334[A]:GLU:OE2	1.81	0.79
2:M:135[A]:ALA:HA	2:M:138[A]:ILE:HD11	1.65	0.79
1:B:392[C]:SER:O	1:B:396[C]:THR:HG22	1.83	0.79
1:J:330[C]:LYS:HE2	1:J:334[C]:GLU:OE2	1.81	0.79
1:E:137[A]:GLN:HE21	1:E:138[A]:VAL:N	1.81	0.79
1:G:442[A]:CYS:HA	1:G:463[A]:ASN:ND2	1.97	0.79
1:I:435[A]:ALA:HB1	1:I:445[A]:ILE:HD11	1.65	0.79
1:D:412[C]:THR:HB	2:L:161[C]:GLU:HG3	1.65	0.79
1:E:137[C]:GLN:HE21	1:E:138[C]:VAL:N	1.81	0.79
1:G:442[C]:CYS:HA	1:G:463[C]:ASN:ND2	1.97	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:435[C]:ALA:HB1	1:I:445[C]:ILE:HD11	1.65	0.79
1:A:430[A]:ASN:HD21	1:B:451[A]:ALA:H	1.29	0.78
1:A:430[C]:ASN:HD21	1:B:451[C]:ALA:H	1.29	0.78
1:I:353[A]:CYS:HB3	1:I:436[A]:LEU:HD23	1.65	0.78
1:E:440[C]:ALA:HA	2:M:155[C]:ARG:NH1	1.98	0.78
1:I:353[C]:CYS:HB3	1:I:436[C]:LEU:HD23	1.65	0.78
1:C:414[A]:ARG:HH11	1:C:414[A]:ARG:HG3	1.48	0.78
1:C:414[C]:ARG:HH11	1:C:414[C]:ARG:HG3	1.48	0.78
1:F:44[A]:THR:HG23	3:F:4755[A]:FAD:O1A	1.82	0.78
3:E:4755[C]:FAD:O1A	1:F:44[C]:THR:HG23	1.82	0.78
1:G:145[A]:LEU:HD23	1:G:316[A]:TYR:HB2	1.62	0.78
1:G:145[C]:LEU:HD23	1:G:316[C]:TYR:HB2	1.62	0.78
2:K:144[A]:LEU:CD1	2:K:166[A]:LEU:HD23	2.14	0.78
2:K:144[A]:LEU:HD13	2:K:166[A]:LEU:CD2	2.14	0.78
1:E:447[A]:ARG:HH11	1:E:447[A]:ARG:CG	1.96	0.78
1:E:447[C]:ARG:HH11	1:E:447[C]:ARG:CG	1.96	0.78
1:B:39[A]:GLU:H	1:B:39[A]:GLU:CD	1.86	0.78
1:I:184[A]:ILE:HG22	1:I:278[A]:ILE:HD11	1.65	0.78
2:K:134[A]:ALA:O	2:K:138[A]:ILE:HG12	1.83	0.78
1:B:39[C]:GLU:CD	1:B:39[C]:GLU:H	1.86	0.78
1:I:184[C]:ILE:HG22	1:I:278[C]:ILE:HD11	1.65	0.78
1:C:325[A]:PRO:O	1:C:330[A]:LYS:HE2	1.84	0.77
2:K:152[A]:THR:HB	2:K:162[A]:ASP:OD1	1.84	0.77
1:C:325[C]:PRO:O	1:C:330[C]:LYS:HE2	1.84	0.77
1:H:370[A]:SER:OG	1:H:373[A]:GLN:HG3	1.84	0.77
1:H:370[C]:SER:OG	1:H:373[C]:GLN:HG3	1.84	0.77
1:H:265[A]:LYS:HB2	1:H:265[A]:LYS:HZ2	1.48	0.77
1:H:265[C]:LYS:HB2	1:H:265[C]:LYS:HZ2	1.48	0.77
2:L:162[C]:ASP:HA	2:L:165[C]:LYS:HG3	1.65	0.77
1:I:82[A]:ARG:HD2	4:I:4772[A]:HOH:O	1.84	0.77
1:I:110[A]:ASN:N	1:I:110[A]:ASN:ND2	2.31	0.77
4:H:4772[C]:HOH:O	1:I:82[C]:ARG:HD2	1.84	0.77
1:I:110[C]:ASN:N	1:I:110[C]:ASN:ND2	2.31	0.77
1:D:82[A]:ARG:NE	1:D:82[A]:ARG:HA	1.97	0.77
1:H:297[A]:ASP:HB2	1:H:298[A]:PRO:HD2	1.66	0.77
1:D:82[C]:ARG:NE	1:D:82[C]:ARG:HA	1.97	0.77
1:H:297[C]:ASP:HB2	1:H:298[C]:PRO:HD2	1.66	0.77
1:C:158[A]:ILE:H	1:C:158[A]:ILE:HD12	1.48	0.77
1:J:301[A]:ARG:HH11	1:J:323[A]:ALA:HA	1.50	0.77
1:C:158[C]:ILE:H	1:C:158[C]:ILE:HD12	1.48	0.77
1:J:301[C]:ARG:HH11	1:J:323[C]:ALA:HA	1.50	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:282[A]:PRO:HG3	1:G:301[A]:ARG:HG2	1.66	0.77
1:G:282[C]:PRO:HG3	1:G:301[C]:ARG:HG2	1.66	0.77
2:M:163[C]:ALA:O	2:M:167[C]:VAL:HG23	1.85	0.77
2:O:158[A]:PHE:HZ	2:O:166[A]:LEU:HD12	1.49	0.76
1:C:45[A]:CYS:HG	1:C:50[A]:CYS:HG	1.31	0.76
1:C:45[C]:CYS:HG	1:C:50[C]:CYS:HG	1.31	0.76
1:E:472[A]:ILE:O	1:E:472[A]:ILE:HD13	1.84	0.76
1:I:23[A]:ILE:HD11	1:I:107[A]:PHE:HD1	1.51	0.76
1:J:259[A]:GLU:HG2	1:J:264[A]:GLY:HA2	1.67	0.76
1:E:472[C]:ILE:O	1:E:472[C]:ILE:HD13	1.84	0.76
1:I:23[C]:ILE:HD11	1:I:107[C]:PHE:HD1	1.51	0.76
1:J:259[C]:GLU:HG2	1:J:264[C]:GLY:HA2	1.67	0.76
1:A:248[A]:LYS:HB2	1:A:248[A]:LYS:HZ2	1.50	0.76
1:F:123[A]:GLY:O	1:F:125[A]:ASN:N	2.19	0.76
1:A:248[C]:LYS:HB2	1:A:248[C]:LYS:HZ2	1.50	0.76
1:F:123[C]:GLY:O	1:F:125[C]:ASN:N	2.19	0.76
1:B:3[A]:GLN:HG2	1:B:4[A]:PRO:CD	2.13	0.76
1:B:3[C]:GLN:HG2	1:B:4[C]:PRO:CD	2.13	0.76
2:M:159[C]:THR:CG2	2:M:162[C]:ASP:H	1.99	0.76
2:K:152[A]:THR:CG2	2:K:153[A]:GLY:H	1.96	0.76
2:L:132[A]:SER:O	2:L:133[A]:PRO:C	2.23	0.76
2:L:142[C]:HIS:O	2:L:144[C]:LEU:HD22	1.86	0.76
1:D:238[A]:LYS:NZ	1:D:269[A]:ILE:HD11	2.01	0.76
1:G:46[A]:LEU:HD12	1:G:46[A]:LEU:O	1.85	0.76
1:D:238[C]:LYS:NZ	1:D:269[C]:ILE:HD11	2.01	0.76
1:G:46[C]:LEU:O	1:G:46[C]:LEU:HD12	1.85	0.76
1:E:451[A]:ALA:H	1:F:430[A]:ASN:HD21	1.32	0.75
1:E:451[C]:ALA:H	1:F:430[C]:ASN:HD21	1.32	0.75
1:D:20[A]:VAL:HG21	1:D:332[A]:GLU:HG3	1.67	0.75
1:D:20[C]:VAL:HG21	1:D:332[C]:GLU:HG3	1.67	0.75
1:D:414[C]:ARG:HD3	2:L:161[C]:GLU:OE2	1.84	0.75
1:C:305[A]:ASN:HB3	1:C:307[A]:ARG:H	1.49	0.75
2:K:130[A]:ARG:HG2	2:K:130[A]:ARG:NH1	2.00	0.75
2:L:151[A]:ALA:HB2	2:L:158[A]:PHE:HA	1.66	0.75
1:C:305[C]:ASN:HB3	1:C:307[C]:ARG:H	1.49	0.75
1:H:124[A]:LYS:H	1:H:124[A]:LYS:CD	1.99	0.75
1:H:124[C]:LYS:H	1:H:124[C]:LYS:CD	1.99	0.75
1:A:434[A]:LEU:HD23	1:B:434[A]:LEU:HD23	1.68	0.75
1:H:155[A]:PHE:CD2	1:H:278[A]:ILE:HD11	2.22	0.75
1:A:434[C]:LEU:HD23	1:B:434[C]:LEU:HD23	1.68	0.75
1:H:155[C]:PHE:CD2	1:H:278[C]:ILE:HD11	2.22	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81[A]:VAL:HG22	1:B:78[A]:MET:HG2	1.68	0.75
1:H:111[A]:LYS:CE	4:H:4823[A]:HOH:O	2.33	0.75
1:J:44[A]:THR:HG23	4:J:4759[A]:FAD:O2A	1.87	0.75
2:L:162[A]:ASP:HA	2:L:165[A]:LYS:HD2	1.67	0.75
1:A:81[C]:VAL:HG22	1:B:78[C]:MET:HG2	1.68	0.75
4:G:4822[C]:HOH:O	1:H:111[C]:LYS:CE	2.33	0.75
1:I:45[C]:CYS:SG	1:I:50[C]:CYS:SG	2.78	0.75
3:I:4759[C]:FAD:O2A	1:J:44[C]:THR:HG23	1.87	0.75
1:C:370[A]:SER:OG	1:C:373[A]:GLN:HG3	1.86	0.75
1:C:370[C]:SER:OG	1:C:373[C]:GLN:HG3	1.86	0.75
1:A:79[A]:SER:CB	1:B:79[A]:SER:HB3	2.17	0.75
2:M:150[A]:THR:HG23	2:M:151[A]:ALA:N	2.00	0.75
1:A:79[C]:SER:CB	1:B:79[C]:SER:HB3	2.17	0.75
1:C:49[A]:GLY:O	1:C:53[A]:SER:HB2	1.86	0.74
1:D:35[A]:ILE:HD11	1:D:139[A]:ILE:HD13	1.68	0.74
1:E:78[A]:MET:H	1:E:78[A]:MET:CE	1.99	0.74
1:I:218[A]:ILE:H	1:I:218[A]:ILE:CD1	1.86	0.74
1:J:406[A]:ILE:HD12	1:J:462[A]:ALA:CB	2.16	0.74
1:C:49[C]:GLY:O	1:C:53[C]:SER:HB2	1.86	0.74
1:D:35[C]:ILE:HD11	1:D:139[C]:ILE:HD13	1.68	0.74
1:E:78[C]:MET:H	1:E:78[C]:MET:CE	1.99	0.74
1:F:443[C]:GLU:OE1	2:M:134[C]:ALA:HB1	1.87	0.74
1:I:218[C]:ILE:H	1:I:218[C]:ILE:CD1	1.86	0.74
1:J:406[C]:ILE:HD12	1:J:462[C]:ALA:CB	2.16	0.74
1:D:238[A]:LYS:HZ3	1:D:269[A]:ILE:HD11	1.52	0.74
1:E:447[A]:ARG:HG2	1:E:447[A]:ARG:NH1	1.94	0.74
1:J:384[A]:GLY:O	1:J:406[A]:ILE:HD13	1.87	0.74
1:D:238[C]:LYS:HZ3	1:D:269[C]:ILE:HD11	1.52	0.74
1:E:447[C]:ARG:HG2	1:E:447[C]:ARG:NH1	1.94	0.74
1:J:384[C]:GLY:O	1:J:406[C]:ILE:HD13	1.87	0.74
1:F:144[A]:ILE:HD12	1:F:145[A]:LEU:N	2.02	0.74
1:F:144[C]:ILE:HD12	1:F:145[C]:LEU:N	2.02	0.74
2:N:136[A]:ARG:CG	2:N:137[A]:ASN:H	2.00	0.74
1:E:137[A]:GLN:HE21	1:E:137[A]:GLN:C	1.89	0.74
1:H:46[A]:LEU:HD21	1:H:100[A]:THR:CG2	2.16	0.74
1:E:137[C]:GLN:HE21	1:E:137[C]:GLN:C	1.89	0.74
1:H:46[C]:LEU:HD21	1:H:100[C]:THR:CG2	2.16	0.74
1:G:7[A]:ALA:HB3	1:G:141[A]:THR:HB	1.67	0.74
2:N:135[A]:ALA:O	2:N:136[A]:ARG:C	2.26	0.74
1:G:7[C]:ALA:HB3	1:G:141[C]:THR:HB	1.67	0.74
1:F:361[A]:HIS:HB2	4:F:4781[A]:HOH:O	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:159[A]:THR:O	2:L:162[A]:ASP:N	2.19	0.74
4:E:4782[C]:HOH:O	1:F:361[C]:HIS:HB2	1.87	0.74
1:B:256[A]:VAL:HG23	1:B:256[A]:VAL:O	1.88	0.74
1:B:256[C]:VAL:O	1:B:256[C]:VAL:HG23	1.88	0.74
1:D:262[A]:SER:OG	1:D:263[A]:GLY:N	2.19	0.74
1:J:239[A]:LEU:O	1:J:241[A]:THR:HG23	1.88	0.74
1:D:262[C]:SER:OG	1:D:263[C]:GLY:N	2.19	0.74
1:J:239[C]:LEU:O	1:J:241[C]:THR:HG23	1.88	0.74
2:L:144[A]:LEU:HD22	2:L:145[A]:ASP:H	1.52	0.73
2:L:155[A]:ARG:HH21	2:L:157[A]:ILE:HG12	1.53	0.73
1:H:318[A]:ILE:HD12	1:H:335[A]:GLY:HA2	1.70	0.73
1:H:318[C]:ILE:HD12	1:H:335[C]:GLY:HA2	1.70	0.73
1:H:82[A]:ARG:HA	1:H:82[A]:ARG:HE	1.53	0.73
1:H:82[C]:ARG:HA	1:H:82[C]:ARG:HE	1.53	0.73
1:A:43[A]:GLY:HA2	3:A:4750[A]:FAD:O3B	1.88	0.73
1:C:290[A]:GLU:H	1:C:290[A]:GLU:CD	1.92	0.73
1:H:461[A]:GLU:OE1	1:H:471[A]:SER:HB2	1.88	0.73
1:A:43[C]:GLY:HA2	3:O:4750[C]:FAD:O3B	1.88	0.73
1:C:290[C]:GLU:H	1:C:290[C]:GLU:CD	1.92	0.73
1:H:461[C]:GLU:OE1	1:H:471[C]:SER:HB2	1.88	0.73
1:H:414[A]:ARG:HG2	1:H:414[A]:ARG:HH11	1.53	0.73
1:H:414[C]:ARG:HG2	1:H:414[C]:ARG:HH11	1.53	0.73
1:I:76[A]:ILE:HD13	1:J:63[A]:TYR:HA	1.71	0.73
1:I:76[C]:ILE:HD13	1:J:63[C]:TYR:HA	1.71	0.73
1:A:455[A]:LEU:H	1:A:455[A]:LEU:HD22	1.54	0.73
1:E:430[A]:ASN:HD21	1:F:451[A]:ALA:H	1.35	0.73
1:F:192[A]:GLU:OE2	4:F:4766[A]:HOH:O	2.07	0.73
1:H:220[A]:MET:HB3	1:H:220[A]:MET:HE2	1.70	0.73
1:I:241[A]:THR:HG22	1:I:260[A]:ALA:HA	1.71	0.73
1:A:455[C]:LEU:H	1:A:455[C]:LEU:HD22	1.54	0.73
1:E:430[C]:ASN:HD21	1:F:451[C]:ALA:H	1.35	0.73
4:E:4766[C]:HOH:O	1:F:192[C]:GLU:OE2	2.07	0.73
1:H:220[C]:MET:HB3	1:H:220[C]:MET:HE2	1.70	0.73
1:I:241[C]:THR:HG22	1:I:260[C]:ALA:HA	1.71	0.73
1:E:27[A]:GLN:HE21	1:E:110[A]:ASN:HD21	1.37	0.72
1:G:339[A]:VAL:HA	1:G:342[A]:MET:HG3	1.71	0.72
1:I:430[A]:ASN:HD21	1:J:451[A]:ALA:H	1.37	0.72
1:E:27[C]:GLN:HE21	1:E:110[C]:ASN:HD21	1.37	0.72
1:G:339[C]:VAL:HA	1:G:342[C]:MET:HG3	1.71	0.72
1:I:430[C]:ASN:HD21	1:J:451[C]:ALA:H	1.37	0.72
1:E:174[A]:LEU:HD12	1:E:197[A]:TRP:CE2	2.24	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:174[C]:LEU:HD12	1:E:197[C]:TRP:CE2	2.24	0.72
1:H:46[A]:LEU:CD2	1:H:100[A]:THR:HG22	2.16	0.72
2:M:142[A]:HIS:HD2	2:M:167[A]:VAL:HG13	1.52	0.72
2:N:136[A]:ARG:CG	2:N:137[A]:ASN:N	2.49	0.72
1:H:46[C]:LEU:CD2	1:H:100[C]:THR:HG22	2.16	0.72
1:C:9[A]:VAL:HG22	1:C:342[A]:MET:HE1	1.69	0.72
1:H:370[A]:SER:H	1:H:373[A]:GLN:HE21	1.36	0.72
1:C:9[C]:VAL:HG22	1:C:342[C]:MET:HE1	1.69	0.72
1:H:370[C]:SER:H	1:H:373[C]:GLN:HE21	1.36	0.72
1:F:181[A]:MET:HE2	1:F:197[A]:TRP:HB2	1.72	0.72
1:F:181[C]:MET:HE2	1:F:197[C]:TRP:HB2	1.72	0.72
2:N:159[C]:THR:HB	2:N:162[C]:ASP:OD2	1.89	0.72
1:D:373[A]:GLN:O	1:D:377[A]:GLU:HG2	1.89	0.72
1:D:373[C]:GLN:O	1:D:377[C]:GLU:HG2	1.89	0.72
2:N:163[C]:ALA:O	2:N:167[C]:VAL:HG23	1.89	0.72
2:N:170[C]:LYS:O	2:N:171[C]:GLN:OE1	2.08	0.72
1:C:44[A]:THR:HG23	3:C:4752[A]:FAD:O1A	1.89	0.72
1:I:292[A]:LEU:O	1:I:294[A]:ILE:HG13	1.89	0.72
2:L:142[A]:HIS:O	2:L:144[A]:LEU:N	2.22	0.72
2:M:152[A]:THR:HG22	2:M:153[A]:GLY:N	2.05	0.72
3:B:4752[C]:FAD:O1A	1:C:44[C]:THR:HG23	1.89	0.72
1:I:292[C]:LEU:O	1:I:294[C]:ILE:HG13	1.89	0.72
2:N:130[C]:ARG:O	2:N:157[C]:ILE:HG23	1.89	0.72
1:G:246[A]:ALA:HB1	1:G:254[A]:ILE:HD11	1.71	0.72
1:I:11[A]:VAL:CG1	1:I:145[A]:LEU:HD23	2.17	0.72
1:G:246[C]:ALA:HB1	1:G:254[C]:ILE:HD11	1.71	0.72
1:I:11[C]:VAL:CG1	1:I:145[C]:LEU:HD23	2.17	0.72
1:B:41[A]:LEU:HD21	1:B:114[A]:HIS:CE1	2.25	0.72
1:C:137[A]:GLN:HE21	1:C:137[A]:GLN:CA	2.02	0.72
1:E:88[A]:MET:CE	1:E:200[A]:LEU:HD21	2.19	0.72
1:B:41[C]:LEU:HD21	1:B:114[C]:HIS:CE1	2.25	0.72
1:C:137[C]:GLN:HE21	1:C:137[C]:GLN:CA	2.02	0.72
1:E:88[C]:MET:CE	1:E:200[C]:LEU:HD21	2.19	0.72
1:G:347[A]:VAL:HG23	1:G:347[A]:VAL:O	1.90	0.71
1:J:468[A]:PHE:HD2	1:J:470[A]:LYS:NZ	1.87	0.71
1:G:347[C]:VAL:HG23	1:G:347[C]:VAL:O	1.90	0.71
1:J:468[C]:PHE:HD2	1:J:470[C]:LYS:NZ	1.87	0.71
2:M:155[A]:ARG:HH21	2:M:157[A]:ILE:CG2	2.03	0.71
2:K:132[C]:SER:O	2:K:134[C]:ALA:N	2.22	0.71
1:E:321[A]:VAL:HG13	1:E:322[A]:VAL:HG23	1.73	0.71
1:J:70[A]:ASP:OD1	1:J:74[A]:ARG:HD2	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:159[A]:THR:OG1	2:L:161[A]:GLU:HB2	1.89	0.71
1:E:321[C]:VAL:HG13	1:E:322[C]:VAL:HG23	1.73	0.71
1:H:438[C]:TYR:HE1	2:N:155[C]:ARG:HD3	1.54	0.71
1:J:70[C]:ASP:OD1	1:J:74[C]:ARG:HD2	1.91	0.71
2:M:145[C]:ASP:O	2:M:148[C]:GLN:CG	2.35	0.71
1:B:444[A]:ASP:OD2	2:K:155[A]:ARG:HD3	1.90	0.71
1:C:151[A]:GLU:OE2	1:C:281[A]:ARG:HD3	1.90	0.71
1:G:54[A]:LYS:HE2	1:G:359[A]:TYR:HD2	1.54	0.71
2:N:131[A]:LEU:HD23	2:N:136[A]:ARG:CA	2.20	0.71
1:C:151[C]:GLU:OE2	1:C:281[C]:ARG:HD3	1.90	0.71
1:G:54[C]:LYS:HE2	1:G:359[C]:TYR:HD2	1.54	0.71
1:H:222[A]:ILE:HG13	1:H:223[A]:SER:N	2.05	0.71
1:H:222[C]:ILE:HG13	1:H:223[C]:SER:N	2.05	0.71
2:K:142[C]:HIS:O	2:K:144[C]:LEU:HG	1.91	0.71
1:A:45[A]:CYS:HG	1:A:50[A]:CYS:HB2	1.55	0.71
1:F:438[A]:TYR:CE1	2:M:133[A]:PRO:HD2	2.25	0.71
1:A:45[C]:CYS:HG	1:A:50[C]:CYS:HB2	1.55	0.71
1:E:88[A]:MET:HE1	1:E:200[A]:LEU:HD21	1.72	0.71
1:G:167[A]:SER:OG	1:G:169[A]:THR:HG22	1.90	0.71
1:I:309[A]:GLN:HB2	4:I:4763[A]:HOH:O	1.89	0.71
1:E:88[C]:MET:HE1	1:E:200[C]:LEU:HD21	1.72	0.71
1:G:167[C]:SER:OG	1:G:169[C]:THR:HG22	1.90	0.71
4:H:4763[C]:HOH:O	1:I:309[C]:GLN:HB2	1.89	0.71
1:I:23[A]:ILE:HD11	1:I:107[A]:PHE:CD1	2.25	0.71
2:N:168[A]:GLN:NE2	2:N:168[A]:GLN:CA	2.41	0.71
1:I:23[C]:ILE:HD11	1:I:107[C]:PHE:CD1	2.25	0.71
2:M:141[C]:LYS:O	2:M:141[C]:LYS:CD	2.38	0.71
1:A:452[A]:HIS:H	1:B:329[A]:HIS:CD2	2.09	0.70
1:I:41[A]:LEU:H	1:I:41[A]:LEU:CD1	2.04	0.70
2:K:171[A]:GLN:O	2:K:173[A]:GLY:N	2.25	0.70
2:L:151[A]:ALA:CB	2:L:162[A]:ASP:OD2	2.38	0.70
2:N:146[A]:ALA:O	2:N:147[A]:SER:C	2.28	0.70
1:A:452[C]:HIS:H	1:B:329[C]:HIS:CD2	2.09	0.70
1:I:41[C]:LEU:H	1:I:41[C]:LEU:CD1	2.04	0.70
1:D:297[A]:ASP:HB2	1:D:298[A]:PRO:HD2	1.73	0.70
1:F:461[A]:GLU:OE1	1:F:471[A]:SER:HB2	1.91	0.70
2:N:142[A]:HIS:HB2	2:N:144[A]:LEU:HD12	1.72	0.70
1:D:297[C]:ASP:HB2	1:D:298[C]:PRO:HD2	1.73	0.70
1:F:461[C]:GLU:OE1	1:F:471[C]:SER:HB2	1.91	0.70
2:M:141[C]:LYS:O	2:M:141[C]:LYS:HD2	1.90	0.70
2:N:167[A]:VAL:O	2:N:171[A]:GLN:HB2	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182[A]:VAL:HG23	1:A:274[A]:LEU:CD1	2.21	0.70
1:A:255[A]:ASP:OD1	1:A:270[A]:THR:HB	1.91	0.70
1:G:267[A]:GLU:HG2	1:G:268[A]:VAL:H	1.55	0.70
1:I:225[A]:ASN:ND2	1:I:228[A]:ARG:HH12	1.90	0.70
1:A:182[C]:VAL:HG23	1:A:274[C]:LEU:CD1	2.21	0.70
1:A:255[C]:ASP:OD1	1:A:270[C]:THR:HB	1.91	0.70
1:G:267[C]:GLU:HG2	1:G:268[C]:VAL:H	1.55	0.70
1:I:225[C]:ASN:ND2	1:I:228[C]:ARG:HH12	1.90	0.70
1:F:437[A]:GLU:HB3	2:M:133[A]:PRO:HG3	1.73	0.70
1:H:397[A]:ASN:HD22	1:H:397[A]:ASN:N	1.88	0.70
1:H:397[C]:ASN:HD22	1:H:397[C]:ASN:N	1.88	0.70
2:N:159[C]:THR:HG21	2:N:161[C]:GLU:HB2	1.74	0.70
1:G:358[A]:ILE:CD1	1:G:360[A]:THR:HG23	2.19	0.70
1:G:358[C]:ILE:CD1	1:G:360[C]:THR:HG23	2.19	0.70
1:E:308[A]:PHE:CE2	1:E:337[A]:ILE:HD11	2.26	0.70
1:I:19[A]:TYR:CE1	1:I:20[A]:VAL:HG12	2.27	0.70
1:E:308[C]:PHE:CE2	1:E:337[C]:ILE:HD11	2.26	0.70
1:I:19[C]:TYR:CE1	1:I:20[C]:VAL:HG12	2.27	0.70
1:F:472[A]:ILE:HD12	1:F:472[A]:ILE:N	2.07	0.70
1:G:431[A]:GLU:OE2	1:G:450[A]:HIS:CE1	2.45	0.70
1:F:472[C]:ILE:HD12	1:F:472[C]:ILE:N	2.07	0.70
1:G:431[C]:GLU:OE2	1:G:450[C]:HIS:CE1	2.45	0.70
1:C:215[A]:GLY:HA3	4:C:4818[A]:HOH:O	1.90	0.70
4:B:4818[C]:HOH:O	1:C:215[C]:GLY:HA3	1.90	0.70
2:K:130[C]:ARG:HD3	2:K:131[C]:LEU:HD22	1.74	0.70
1:B:305[A]:ASN:ND2	1:B:307[A]:ARG:H	1.90	0.69
1:I:10[A]:THR:HG23	1:I:33[A]:VAL:HG13	1.72	0.69
1:B:305[C]:ASN:ND2	1:B:307[C]:ARG:H	1.90	0.69
1:I:10[C]:THR:HG23	1:I:33[C]:VAL:HG13	1.72	0.69
1:B:256[A]:VAL:HG22	1:B:269[A]:ILE:O	1.92	0.69
1:E:27[A]:GLN:HE21	1:E:110[A]:ASN:ND2	1.90	0.69
1:B:256[C]:VAL:HG22	1:B:269[C]:ILE:O	1.92	0.69
1:E:27[C]:GLN:HE21	1:E:110[C]:ASN:ND2	1.90	0.69
2:K:155[C]:ARG:O	2:K:155[C]:ARG:HG2	1.92	0.69
1:F:229[A]:ILE:HG21	1:F:362[A]:PRO:HG3	1.72	0.69
1:J:37[A]:LYS:HE3	4:J:4759[A]:FAD:C4A	2.22	0.69
2:M:131[A]:LEU:CD1	2:M:136[A]:ARG:HH21	2.05	0.69
1:F:229[C]:ILE:HG21	1:F:362[C]:PRO:HG3	1.72	0.69
3:I:4759[C]:FAD:C4A	1:J:37[C]:LYS:HE3	2.22	0.69
1:E:448[A]:VAL:HG22	1:F:437[A]:GLU:HG3	1.74	0.69
1:A:348[C]:HIS:HB2	2:K:140[C]:GLU:OE2	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:448[C]:VAL:HG22	1:F:437[C]:GLU:HG3	1.74	0.69
1:I:138[A]:VAL:C	1:I:139[A]:ILE:HD12	2.12	0.69
2:K:171[A]:GLN:H	2:K:171[A]:GLN:CD	1.95	0.69
1:D:443[C]:GLU:HG2	2:L:134[C]:ALA:HB2	1.74	0.69
1:I:138[C]:VAL:C	1:I:139[C]:ILE:HD12	2.12	0.69
1:C:452[A]:HIS:CD2	1:C:453[A]:PRO:HB3	2.28	0.69
1:H:111[A]:LYS:HE2	4:H:4823[A]:HOH:O	1.90	0.69
1:H:442[A]:CYS:HB2	1:H:467[A]:SER:HB2	1.73	0.69
1:C:452[C]:HIS:CD2	1:C:453[C]:PRO:HB3	2.28	0.69
4:G:4822[C]:HOH:O	1:H:111[C]:LYS:HE2	1.90	0.69
1:H:442[C]:CYS:HB2	1:H:467[C]:SER:HB2	1.73	0.69
2:N:131[C]:LEU:CD2	2:N:146[C]:ALA:HB2	2.23	0.69
1:A:79[A]:SER:HB3	1:B:79[A]:SER:CB	2.22	0.69
1:A:92[A]:LYS:HG3	1:A:93[A]:SER:N	2.05	0.69
1:G:51[A]:ILE:HG23	1:H:396[A]:THR:HG21	1.73	0.69
1:G:145[A]:LEU:HD21	1:G:338[A]:CYS:SG	2.32	0.69
1:G:180[A]:LYS:HG2	1:G:203[A]:ASP:HB3	1.74	0.69
1:A:79[C]:SER:HB3	1:B:79[C]:SER:CB	2.22	0.69
1:A:92[C]:LYS:HG3	1:A:93[C]:SER:N	2.05	0.69
1:G:51[C]:ILE:HG23	1:H:396[C]:THR:HG21	1.73	0.69
1:G:145[C]:LEU:HD21	1:G:338[C]:CYS:SG	2.32	0.69
1:G:180[C]:LYS:HG2	1:G:203[C]:ASP:HB3	1.74	0.69
1:C:44[A]:THR:CG2	3:C:4752[A]:FAD:O2A	2.41	0.69
1:C:358[A]:ILE:C	1:C:358[A]:ILE:HD12	2.13	0.69
1:C:473[A]:ASN:HA	1:D:106[A]:LEU:HD21	1.75	0.69
1:E:54[A]:LYS:HE2	1:E:359[A]:TYR:CD1	2.27	0.69
1:F:305[A]:ASN:ND2	1:F:309[A]:GLN:HG3	2.08	0.69
1:G:256[A]:VAL:O	1:G:256[A]:VAL:HG23	1.92	0.69
1:H:305[A]:ASN:ND2	1:H:307[A]:ARG:H	1.90	0.69
2:M:159[A]:THR:HG21	2:M:161[A]:GLU:HB2	1.74	0.69
3:B:4752[C]:FAD:O2A	1:C:44[C]:THR:CG2	2.41	0.69
1:C:358[C]:ILE:C	1:C:358[C]:ILE:HD12	2.13	0.69
1:C:473[C]:ASN:HA	1:D:106[C]:LEU:HD21	1.75	0.69
1:E:54[C]:LYS:HE2	1:E:359[C]:TYR:CD1	2.27	0.69
1:F:305[C]:ASN:ND2	1:F:309[C]:GLN:HG3	2.08	0.69
1:G:256[C]:VAL:HG23	1:G:256[C]:VAL:O	1.92	0.69
1:H:305[C]:ASN:ND2	1:H:307[C]:ARG:H	1.90	0.69
1:B:320[A]:ASP:HB3	4:B:4801[A]:HOH:O	1.93	0.69
1:F:256[A]:VAL:HG23	1:F:269[A]:ILE:HB	1.75	0.69
1:I:383[A]:VAL:HG23	1:I:407[A]:LEU:HD23	1.73	0.69
4:A:4801[C]:HOH:O	1:B:320[C]:ASP:HB3	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:256[C]:VAL:HG23	1:F:269[C]:ILE:HB	1.75	0.69
1:I:383[C]:VAL:HG23	1:I:407[C]:LEU:HD23	1.73	0.69
1:F:305[A]:ASN:HD21	1:F:309[A]:GLN:HG3	1.57	0.69
1:H:124[A]:LYS:HD3	1:H:124[A]:LYS:N	2.04	0.69
1:H:219[A]:ASP:HB3	1:H:222[A]:ILE:HG12	1.74	0.69
2:L:145[A]:ASP:OD1	2:L:147[A]:SER:HB2	1.93	0.69
1:F:305[C]:ASN:HD21	1:F:309[C]:GLN:HG3	1.57	0.69
1:H:124[C]:LYS:HD3	1:H:124[C]:LYS:N	2.04	0.69
1:H:219[C]:ASP:HB3	1:H:222[C]:ILE:HG12	1.74	0.69
1:B:133[A]:ASP:O	1:B:135[A]:GLY:N	2.25	0.68
1:D:1[A]:ALA:HA	1:D:136[A]:THR:HG23	1.76	0.68
2:L:142[A]:HIS:O	2:L:144[A]:LEU:HB2	1.92	0.68
2:L:144[A]:LEU:CD1	2:L:166[A]:LEU:HB3	2.19	0.68
1:B:133[C]:ASP:O	1:B:135[C]:GLY:N	2.25	0.68
1:D:1[C]:ALA:HA	1:D:136[C]:THR:HG23	1.76	0.68
1:G:84[A]:ASN:C	1:G:84[A]:ASN:HD22	1.94	0.68
1:G:84[C]:ASN:C	1:G:84[C]:ASN:HD22	1.94	0.68
2:K:149[C]:GLY:HA3	2:K:166[C]:LEU:HD21	1.73	0.68
1:C:414[A]:ARG:HH11	1:C:414[A]:ARG:HG2	1.57	0.68
1:H:373[A]:GLN:HB3	4:H:4787[A]:HOH:O	1.92	0.68
1:H:431[A]:GLU:OE2	1:H:450[A]:HIS:HE1	1.75	0.68
1:J:415[A]:VAL:HG22	1:J:440[A]:ALA:O	1.92	0.68
2:K:159[A]:THR:HG22	2:K:160[A]:LYS:N	2.07	0.68
1:C:414[C]:ARG:HH11	1:C:414[C]:ARG:HG2	1.57	0.68
4:G:4787[C]:HOH:O	1:H:373[C]:GLN:HB3	1.92	0.68
1:H:431[C]:GLU:OE2	1:H:450[C]:HIS:HE1	1.75	0.68
1:J:415[C]:VAL:HG22	1:J:440[C]:ALA:O	1.92	0.68
1:A:84[A]:ASN:ND2	1:A:87[A]:LYS:H	1.92	0.68
1:E:312[A]:ILE:HD13	1:E:313[A]:PRO:N	2.08	0.68
1:F:181[A]:MET:CE	1:F:197[A]:TRP:HB2	2.23	0.68
1:G:297[A]:ASP:HB3	1:G:299[A]:ARG:H	1.56	0.68
1:A:84[C]:ASN:ND2	1:A:87[C]:LYS:H	1.92	0.68
1:E:312[C]:ILE:HD13	1:E:313[C]:PRO:N	2.08	0.68
1:F:181[C]:MET:CE	1:F:197[C]:TRP:HB2	2.23	0.68
1:G:297[C]:ASP:HB3	1:G:299[C]:ARG:H	1.56	0.68
1:B:155[A]:PHE:CZ	1:B:243[A]:VAL:HG13	2.28	0.68
1:B:155[C]:PHE:CZ	1:B:243[C]:VAL:HG13	2.28	0.68
2:M:154[C]:PRO:O	2:M:156[C]:GLY:N	2.27	0.68
1:H:82[A]:ARG:HA	1:H:82[A]:ARG:NE	2.09	0.68
1:J:353[A]:CYS:SG	1:J:436[A]:LEU:HB3	2.34	0.68
2:K:137[A]:ASN:HD22	2:K:138[A]:ILE:N	1.90	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:162[A]:ASP:HA	2:O:165[A]:LYS:HD3	1.75	0.68
1:H:82[C]:ARG:HA	1:H:82[C]:ARG:NE	2.09	0.68
1:J:353[C]:CYS:SG	1:J:436[C]:LEU:HB3	2.34	0.68
2:M:131[C]:LEU:HD22	2:M:136[C]:ARG:HB2	1.76	0.68
1:I:20[A]:VAL:HG11	1:I:332[A]:GLU:HG2	1.74	0.68
1:I:307[A]:ARG:HG2	1:I:347[A]:VAL:HG21	1.75	0.68
1:I:20[C]:VAL:HG11	1:I:332[C]:GLU:HG2	1.74	0.68
1:I:307[C]:ARG:HG2	1:I:347[C]:VAL:HG21	1.75	0.68
1:A:347[A]:VAL:HG23	1:A:347[A]:VAL:O	1.94	0.68
1:E:308[A]:PHE:HE2	1:E:337[A]:ILE:HD11	1.58	0.68
1:E:409[A]:GLN:HE21	1:E:411[A]:SER:N	1.91	0.68
1:I:45[A]:CYS:CB	1:I:50[A]:CYS:HG	2.06	0.68
2:N:139[A]:LEU:HD11	2:N:158[A]:PHE:CE2	2.29	0.68
2:O:155[A]:ARG:N	2:O:157[A]:ILE:HD11	2.08	0.68
1:A:45[C]:CYS:SG	1:A:50[C]:CYS:SG	2.79	0.68
1:A:347[C]:VAL:HG23	1:A:347[C]:VAL:O	1.94	0.68
1:E:308[C]:PHE:HE2	1:E:337[C]:ILE:HD11	1.58	0.68
1:E:409[C]:GLN:HE21	1:E:411[C]:SER:N	1.91	0.68
1:I:45[C]:CYS:CB	1:I:50[C]:CYS:HG	2.06	0.68
1:J:305[A]:ASN:ND2	1:J:309[A]:GLN:HG3	2.09	0.68
1:J:409[A]:GLN:NE2	1:J:412[A]:THR:OG1	2.27	0.68
1:J:305[C]:ASN:ND2	1:J:309[C]:GLN:HG3	2.09	0.68
1:J:409[C]:GLN:NE2	1:J:412[C]:THR:OG1	2.27	0.68
1:G:453[A]:PRO:HA	1:G:457[A]:GLU:OE2	1.93	0.68
1:I:78[A]:MET:HG2	1:J:78[A]:MET:HG2	1.75	0.68
2:O:131[A]:LEU:CD2	2:O:135[A]:ALA:HB3	2.23	0.68
1:G:453[C]:PRO:HA	1:G:457[C]:GLU:OE2	1.93	0.68
1:I:78[C]:MET:HG2	1:J:78[C]:MET:HG2	1.75	0.68
1:C:307[A]:ARG:HA	1:C:347[A]:VAL:HG21	1.74	0.67
1:C:307[C]:ARG:HA	1:C:347[C]:VAL:HG21	1.74	0.67
1:C:192[A]:GLU:OE1	4:C:4823[A]:HOH:O	2.12	0.67
1:I:297[A]:ASP:HB3	1:I:299[A]:ARG:H	1.58	0.67
4:B:4823[C]:HOH:O	1:C:192[C]:GLU:OE1	2.12	0.67
1:I:297[C]:ASP:HB3	1:I:299[C]:ARG:H	1.58	0.67
2:N:159[C]:THR:HG22	2:N:161[C]:GLU:N	2.09	0.67
1:G:137[A]:GLN:HE21	1:G:138[A]:VAL:N	1.90	0.67
1:G:137[C]:GLN:HE21	1:G:138[C]:VAL:N	1.90	0.67
2:K:132[C]:SER:O	2:K:133[C]:PRO:C	2.31	0.67
1:F:146[A]:ILE:HG22	1:F:148[A]:THR:HG23	1.77	0.67
1:H:143[A]:ASN:HB2	1:H:342[A]:MET:HE1	1.75	0.67
1:I:464[A]:LEU:HD23	1:I:471[A]:SER:HA	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:122[A]:THR:HG21	1:J:128[A]:THR:HG21	1.75	0.67
1:F:146[C]:ILE:HG22	1:F:148[C]:THR:HG23	1.77	0.67
1:H:143[C]:ASN:HB2	1:H:342[C]:MET:HE1	1.75	0.67
1:I:464[C]:LEU:HD23	1:I:471[C]:SER:HA	1.75	0.67
1:J:122[C]:THR:HG21	1:J:128[C]:THR:HG21	1.75	0.67
1:A:14[A]:SER:HB3	1:A:36[A]:GLU:HB2	1.77	0.67
1:A:14[C]:SER:HB3	1:A:36[C]:GLU:HB2	1.77	0.67
1:A:289[A]:LEU:HA	1:A:292[A]:LEU:HD12	1.77	0.67
1:F:1[A]:ALA:N	1:F:136[A]:THR:HG22	2.10	0.67
1:J:44[A]:THR:HG23	4:J:4759[A]:FAD:PA	2.34	0.67
1:J:393[A]:ARG:HB3	1:J:455[A]:LEU:HD13	1.76	0.67
1:A:289[C]:LEU:HA	1:A:292[C]:LEU:HD12	1.77	0.67
1:F:1[C]:ALA:N	1:F:136[C]:THR:HG22	2.10	0.67
3:I:4759[C]:FAD:PA	1:J:44[C]:THR:HG23	2.34	0.67
1:J:393[C]:ARG:HB3	1:J:455[C]:LEU:HD13	1.76	0.67
1:C:286[A]:ASN:OD1	4:C:4774[A]:HOH:O	2.13	0.67
1:H:10[A]:THR:HG21	1:H:139[A]:ILE:HG21	1.76	0.67
4:B:4774[C]:HOH:O	1:C:286[C]:ASN:OD1	2.13	0.67
1:H:10[C]:THR:HG21	1:H:139[C]:ILE:HG21	1.76	0.67
1:A:358[A]:ILE:HD12	1:A:360[A]:THR:HG23	1.75	0.67
1:B:432[A]:ALA:O	1:B:436[A]:LEU:HD23	1.94	0.67
1:D:69[A]:LYS:HG3	1:D:69[A]:LYS:O	1.93	0.67
1:A:358[C]:ILE:HD12	1:A:360[C]:THR:HG23	1.75	0.67
1:B:432[C]:ALA:O	1:B:436[C]:LEU:HD23	1.94	0.67
1:D:69[C]:LYS:HG3	1:D:69[C]:LYS:O	1.93	0.67
1:A:44[A]:THR:HG23	3:A:4750[A]:FAD:O1A	1.95	0.67
1:G:431[A]:GLU:OE2	1:G:450[A]:HIS:HE1	1.77	0.67
1:H:414[A]:ARG:HG2	1:H:414[A]:ARG:NH1	2.09	0.67
1:A:44[C]:THR:HG23	3:O:4750[C]:FAD:O1A	1.95	0.67
1:G:431[C]:GLU:OE2	1:G:450[C]:HIS:HE1	1.77	0.67
1:H:414[C]:ARG:HG2	1:H:414[C]:ARG:NH1	2.09	0.67
1:B:144[A]:ILE:HD12	1:B:145[A]:LEU:N	2.10	0.67
1:D:33[A]:VAL:HB	1:D:113[A]:VAL:HB	1.77	0.67
1:J:392[A]:SER:O	1:J:396[A]:THR:HB	1.95	0.67
1:B:144[C]:ILE:HD12	1:B:145[C]:LEU:N	2.10	0.67
1:D:33[C]:VAL:HB	1:D:113[C]:VAL:HB	1.77	0.67
1:J:392[C]:SER:O	1:J:396[C]:THR:HB	1.95	0.67
1:A:427[A]:GLU:OE2	1:B:454[A]:THR:HB	1.95	0.66
1:E:312[A]:ILE:C	1:E:312[A]:ILE:CD1	2.64	0.66
1:G:248[A]:LYS:H	1:G:248[A]:LYS:CD	2.07	0.66
1:J:289[A]:LEU:CD2	1:J:294[A]:ILE:HD12	2.23	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:427[C]:GLU:OE2	1:B:454[C]:THR:HB	1.95	0.66
1:E:312[C]:ILE:C	1:E:312[C]:ILE:CD1	2.64	0.66
1:G:248[C]:LYS:CD	1:G:248[C]:LYS:H	2.07	0.66
1:J:289[C]:LEU:CD2	1:J:294[C]:ILE:HD12	2.23	0.66
2:L:151[C]:ALA:HB1	2:L:162[C]:ASP:OD2	1.94	0.66
1:A:447[A]:ARG:NH2	2:K:137[A]:ASN:OD1	2.28	0.66
1:B:380[A]:GLU:HG2	1:J:84[A]:ASN:ND2	2.10	0.66
1:C:121[A]:ILE:HG21	1:C:292[A]:LEU:HD11	1.77	0.66
1:D:69[A]:LYS:HD2	1:D:72[A]:ALA:HB3	1.77	0.66
1:E:248[A]:LYS:HE3	1:E:252[A]:GLY:O	1.95	0.66
1:F:155[A]:PHE:CD1	1:F:158[A]:ILE:HG13	2.29	0.66
1:G:82[A]:ARG:NE	1:G:82[A]:ARG:HA	2.09	0.66
1:B:380[C]:GLU:HG2	1:J:84[C]:ASN:ND2	2.10	0.66
1:C:121[C]:ILE:HG21	1:C:292[C]:LEU:HD11	1.77	0.66
1:D:69[C]:LYS:HD2	1:D:72[C]:ALA:HB3	1.77	0.66
1:E:248[C]:LYS:HE3	1:E:252[C]:GLY:O	1.95	0.66
1:F:155[C]:PHE:CD1	1:F:158[C]:ILE:HG13	2.29	0.66
1:G:82[C]:ARG:NE	1:G:82[C]:ARG:HA	2.09	0.66
2:N:152[C]:THR:HG22	2:N:153[C]:GLY:H	1.59	0.66
1:B:428[A]:MET:CE	1:B:459[A]:PHE:HB2	2.26	0.66
1:H:121[A]:ILE:CD1	1:H:144[A]:ILE:HD11	2.25	0.66
1:B:428[C]:MET:CE	1:B:459[C]:PHE:HB2	2.26	0.66
1:H:121[C]:ILE:CD1	1:H:144[C]:ILE:HD11	2.25	0.66
2:N:159[C]:THR:HG22	2:N:161[C]:GLU:H	1.59	0.66
1:I:336[A]:ILE:HG22	1:I:337[A]:ILE:HG23	1.77	0.66
1:I:336[C]:ILE:HG22	1:I:337[C]:ILE:HG23	1.77	0.66
1:B:20[A]:VAL:HG21	1:B:332[A]:GLU:HG2	1.77	0.66
2:K:159[A]:THR:CG2	2:K:160[A]:LYS:N	2.58	0.66
1:B:20[C]:VAL:HG21	1:B:332[C]:GLU:HG2	1.77	0.66
1:B:330[A]:LYS:HE2	1:B:334[A]:GLU:OE2	1.94	0.66
1:G:259[A]:GLU:OE2	1:G:264[A]:GLY:HA2	1.95	0.66
1:B:330[C]:LYS:HE2	1:B:334[C]:GLU:OE2	1.94	0.66
1:G:259[C]:GLU:OE2	1:G:264[C]:GLY:HA2	1.95	0.66
1:A:248[A]:LYS:HB2	1:A:248[A]:LYS:NZ	2.09	0.66
1:E:312[A]:ILE:HG23	1:E:315[A]:ILE:HB	1.76	0.66
1:H:187[A]:GLY:O	1:H:191[A]:VAL:HG22	1.96	0.66
2:N:133[A]:PRO:CA	2:N:136[A]:ARG:HE	2.05	0.66
1:A:248[C]:LYS:HB2	1:A:248[C]:LYS:NZ	2.09	0.66
1:E:312[C]:ILE:HG23	1:E:315[C]:ILE:HB	1.76	0.66
1:H:187[C]:GLY:O	1:H:191[C]:VAL:HG22	1.96	0.66
2:L:151[C]:ALA:HB2	2:L:162[C]:ASP:HB2	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:364[A]:VAL:HG22	1:A:421[A]:LEU:HD13	1.78	0.66
1:A:364[C]:VAL:HG22	1:A:421[C]:LEU:HD13	1.78	0.66
1:A:363[A]:GLU:HB2	1:A:425[A]:ALA:HB3	1.77	0.66
1:D:183[A]:VAL:HG13	1:D:275[A]:LEU:HB3	1.77	0.66
1:F:50[A]:CYS:O	1:F:54[A]:LYS:HE2	1.95	0.66
2:M:131[A]:LEU:CD1	2:M:136[A]:ARG:NE	2.47	0.66
2:M:152[A]:THR:N	2:M:162[A]:ASP:OD2	2.28	0.66
1:A:363[C]:GLU:HB2	1:A:425[C]:ALA:HB3	1.77	0.66
1:D:183[C]:VAL:HG13	1:D:275[C]:LEU:HB3	1.77	0.66
1:F:50[C]:CYS:O	1:F:54[C]:LYS:HE2	1.95	0.66
2:K:139[C]:LEU:HD23	2:K:163[C]:ALA:HB1	1.78	0.66
1:B:137[A]:GLN:NE2	1:B:138[A]:VAL:N	2.44	0.66
1:B:137[C]:GLN:NE2	1:B:138[C]:VAL:N	2.44	0.66
1:A:182[A]:VAL:HG23	1:A:274[A]:LEU:HD12	1.78	0.65
1:A:406[A]:ILE:HG21	1:A:463[A]:ASN:ND2	2.11	0.65
1:A:182[C]:VAL:HG23	1:A:274[C]:LEU:HD12	1.78	0.65
1:A:406[C]:ILE:HG21	1:A:463[C]:ASN:ND2	2.11	0.65
2:K:142[C]:HIS:O	2:K:143[C]:SER:C	2.34	0.65
1:B:363[A]:GLU:HB3	1:B:425[A]:ALA:HB3	1.78	0.65
1:E:14[A]:SER:O	1:E:19[A]:TYR:HB3	1.96	0.65
1:G:434[A]:LEU:HD13	1:H:448[A]:VAL:HG21	1.77	0.65
1:B:363[C]:GLU:HB3	1:B:425[C]:ALA:HB3	1.78	0.65
1:E:14[C]:SER:O	1:E:19[C]:TYR:HB3	1.96	0.65
1:G:434[C]:LEU:HD13	1:H:448[C]:VAL:HG21	1.77	0.65
1:E:464[A]:LEU:O	1:E:464[A]:LEU:HD23	1.97	0.65
1:J:155[A]:PHE:CZ	1:J:243[A]:VAL:HG22	2.31	0.65
1:E:464[C]:LEU:O	1:E:464[C]:LEU:HD23	1.97	0.65
1:J:155[C]:PHE:CZ	1:J:243[C]:VAL:HG22	2.31	0.65
1:B:370[A]:SER:OG	1:B:373[A]:GLN:HG3	1.96	0.65
1:C:305[A]:ASN:HB2	1:C:309[A]:GLN:H	1.61	0.65
1:J:51[A]:ILE:HB	1:J:52[A]:PRO:CD	2.23	0.65
2:M:150[A]:THR:HG22	2:M:151[A]:ALA:N	2.11	0.65
1:B:370[C]:SER:OG	1:B:373[C]:GLN:HG3	1.96	0.65
1:C:305[C]:ASN:HB2	1:C:309[C]:GLN:H	1.61	0.65
1:J:51[C]:ILE:HB	1:J:52[C]:PRO:CD	2.23	0.65
1:F:48[A]:VAL:HG23	1:F:48[A]:VAL:O	1.97	0.65
1:I:301[A]:ARG:HH11	1:I:323[A]:ALA:HA	1.61	0.65
1:F:48[C]:VAL:HG23	1:F:48[C]:VAL:O	1.97	0.65
1:I:301[C]:ARG:HH11	1:I:323[C]:ALA:HA	1.61	0.65
2:M:167[A]:VAL:O	2:M:170[A]:LYS:HG3	1.96	0.65
1:A:371[A]:GLU:HG2	1:A:381[A]:TYR:OH	1.94	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:318[A]:ILE:HD12	1:C:335[A]:GLY:CA	2.26	0.65
1:F:121[A]:ILE:HD11	1:F:146[A]:ILE:HD11	1.79	0.65
1:I:41[A]:LEU:HD12	1:I:41[A]:LEU:N	2.06	0.65
1:A:371[C]:GLU:HG2	1:A:381[C]:TYR:OH	1.94	0.65
1:C:318[C]:ILE:HD12	1:C:335[C]:GLY:CA	2.26	0.65
1:F:121[C]:ILE:HD11	1:F:146[C]:ILE:HD11	1.79	0.65
1:I:41[C]:LEU:HD12	1:I:41[C]:LEU:N	2.06	0.65
1:A:137[A]:GLN:HE21	1:A:138[A]:VAL:N	1.95	0.65
1:H:121[A]:ILE:HD11	1:H:144[A]:ILE:HD11	1.78	0.65
1:A:137[C]:GLN:HE21	1:A:138[C]:VAL:N	1.95	0.65
1:H:121[C]:ILE:HD11	1:H:144[C]:ILE:HD11	1.78	0.65
1:J:409[A]:GLN:HB2	1:J:416[A]:LEU:HD21	1.79	0.65
1:J:409[C]:GLN:HB2	1:J:416[C]:LEU:HD21	1.79	0.65
1:A:238[A]:LYS:CA	1:A:238[A]:LYS:HE3	2.26	0.65
1:C:182[A]:VAL:HG13	1:C:271[A]:CYS:SG	2.37	0.65
1:D:183[A]:VAL:HG13	1:D:275[A]:LEU:HD13	1.78	0.65
1:G:299[A]:ARG:H	1:G:299[A]:ARG:HD2	1.61	0.65
1:A:238[C]:LYS:CA	1:A:238[C]:LYS:HE3	2.26	0.65
1:C:182[C]:VAL:HG13	1:C:271[C]:CYS:SG	2.37	0.65
1:D:183[C]:VAL:HG13	1:D:275[C]:LEU:HD13	1.78	0.65
1:G:299[C]:ARG:H	1:G:299[C]:ARG:HD2	1.61	0.65
2:M:141[C]:LYS:HD2	2:M:141[C]:LYS:C	2.17	0.65
1:I:337[A]:ILE:HA	1:I:340[A]:GLU:HB2	1.78	0.64
1:I:337[C]:ILE:HA	1:I:340[C]:GLU:HB2	1.78	0.64
1:A:438[A]:TYR:C	2:K:154[A]:PRO:HG3	2.17	0.64
2:M:131[A]:LEU:HB2	2:M:136[A]:ARG:HB2	1.79	0.64
1:D:145[A]:LEU:HD21	1:D:318[A]:ILE:HD12	1.78	0.64
1:F:15[A]:GLY:HA2	1:F:43[A]:GLY:HA3	1.78	0.64
1:H:290[A]:GLU:H	1:H:290[A]:GLU:CD	2.01	0.64
1:I:184[A]:ILE:HG22	1:I:278[A]:ILE:CD1	2.27	0.64
1:C:45[C]:CYS:SG	1:C:50[C]:CYS:SG	2.91	0.64
1:D:145[C]:LEU:HD21	1:D:318[C]:ILE:HD12	1.78	0.64
1:F:15[C]:GLY:HA2	1:F:43[C]:GLY:HA3	1.78	0.64
1:H:290[C]:GLU:H	1:H:290[C]:GLU:CD	2.01	0.64
1:I:184[C]:ILE:HG22	1:I:278[C]:ILE:CD1	2.27	0.64
1:E:188[A]:VAL:HG22	1:E:358[A]:ILE:HD13	1.79	0.64
1:H:96[A]:VAL:O	1:H:100[A]:THR:HG23	1.98	0.64
1:H:189[A]:ILE:HB	4:H:4802[A]:HOH:O	1.97	0.64
1:J:280[A]:ARG:HH11	1:J:280[A]:ARG:CG	2.10	0.64
2:K:159[A]:THR:CG2	2:K:161[A]:GLU:H	2.06	0.64
1:E:188[C]:VAL:HG22	1:E:358[C]:ILE:HD13	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:4802[C]:HOH:O	1:H:189[C]:ILE:HB	1.97	0.64
1:H:96[C]:VAL:O	1:H:100[C]:THR:HG23	1.98	0.64
1:J:280[C]:ARG:HH11	1:J:280[C]:ARG:CG	2.10	0.64
1:D:369[A]:LYS:HE2	1:D:377[A]:GLU:OE2	1.97	0.64
1:E:137[A]:GLN:CA	1:E:137[A]:GLN:NE2	2.58	0.64
1:E:305[A]:ASN:ND2	1:E:309[A]:GLN:H	1.95	0.64
1:D:369[C]:LYS:HE2	1:D:377[C]:GLU:OE2	1.97	0.64
1:E:137[C]:GLN:CA	1:E:137[C]:GLN:NE2	2.58	0.64
1:E:305[C]:ASN:ND2	1:E:309[C]:GLN:H	1.95	0.64
1:H:122[A]:THR:OG1	1:H:126[A]:GLN:HG2	1.97	0.64
1:H:165[A]:ILE:HD11	1:H:254[A]:ILE:HD12	1.79	0.64
2:O:155[A]:ARG:H	2:O:157[A]:ILE:HD11	1.60	0.64
1:H:122[C]:THR:OG1	1:H:126[C]:GLN:HG2	1.97	0.64
1:H:165[C]:ILE:HD11	1:H:254[C]:ILE:HD12	1.79	0.64
1:E:372[A]:GLU:O	1:E:376[A]:GLU:HG3	1.98	0.64
1:H:305[A]:ASN:C	1:H:305[A]:ASN:ND2	2.51	0.64
1:J:122[A]:THR:CG2	1:J:128[A]:THR:CG2	2.75	0.64
1:E:372[C]:GLU:O	1:E:376[C]:GLU:HG3	1.98	0.64
1:H:305[C]:ASN:C	1:H:305[C]:ASN:ND2	2.51	0.64
1:J:122[C]:THR:CG2	1:J:128[C]:THR:CG2	2.75	0.64
1:H:143[A]:ASN:CB	1:H:342[A]:MET:HE1	2.26	0.64
2:O:155[A]:ARG:O	2:O:155[A]:ARG:HD2	1.97	0.64
1:H:143[C]:ASN:CB	1:H:342[C]:MET:HE1	2.26	0.64
2:N:159[C]:THR:HG22	2:N:161[C]:GLU:CB	2.28	0.64
1:E:174[A]:LEU:HD12	1:E:197[A]:TRP:CZ2	2.33	0.64
1:E:182[A]:VAL:HG13	1:E:271[A]:CYS:SG	2.38	0.64
1:E:174[C]:LEU:HD12	1:E:197[C]:TRP:CZ2	2.33	0.64
1:E:182[C]:VAL:HG13	1:E:271[C]:CYS:SG	2.38	0.64
2:K:155[C]:ARG:O	2:K:155[C]:ARG:CG	2.43	0.64
1:D:187[A]:GLY:O	1:D:191[A]:VAL:HG23	1.98	0.64
1:E:305[A]:ASN:C	1:E:305[A]:ASN:HD22	2.00	0.64
1:J:305[A]:ASN:ND2	1:J:309[A]:GLN:CG	2.61	0.64
1:D:187[C]:GLY:O	1:D:191[C]:VAL:HG23	1.98	0.64
1:E:305[C]:ASN:C	1:E:305[C]:ASN:HD22	2.00	0.64
1:J:305[C]:ASN:ND2	1:J:309[C]:GLN:CG	2.61	0.64
1:E:188[A]:VAL:HG22	1:E:358[A]:ILE:HD11	1.78	0.63
1:I:24[A]:LYS:O	1:I:24[A]:LYS:HD3	1.98	0.63
1:E:188[C]:VAL:HG22	1:E:358[C]:ILE:HD11	1.78	0.63
1:I:24[C]:LYS:O	1:I:24[C]:LYS:HD3	1.98	0.63
1:D:320[A]:ASP:OD2	3:D:4753[A]:FAD:H5'1	1.98	0.63
1:H:45[A]:CYS:HG	1:H:50[A]:CYS:HG	1.44	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:188[A]:VAL:HG13	1:H:358[A]:ILE:HG23	1.78	0.63
3:C:4753[C]:FAD:H5'1	1:D:320[C]:ASP:OD2	1.98	0.63
1:H:45[C]:CYS:HG	1:H:50[C]:CYS:HG	1.44	0.63
1:H:188[C]:VAL:HG13	1:H:358[C]:ILE:HG23	1.78	0.63
1:B:180[A]:LYS:HB2	1:B:180[A]:LYS:NZ	2.14	0.63
1:C:451[A]:ALA:H	1:D:430[A]:ASN:HD21	1.46	0.63
1:B:180[C]:LYS:NZ	1:B:180[C]:LYS:HB2	2.14	0.63
1:C:451[C]:ALA:H	1:D:430[C]:ASN:HD21	1.46	0.63
1:B:189[A]:ILE:HG23	3:B:4751[A]:FAD:HM73	1.81	0.63
1:J:461[A]:GLU:OE1	1:J:471[A]:SER:HB2	1.98	0.63
3:A:4751[C]:FAD:HM73	1:B:189[C]:ILE:HG23	1.81	0.63
1:G:437[C]:GLU:HG3	2:N:136[C]:ARG:HH22	1.64	0.63
1:J:461[C]:GLU:OE1	1:J:471[C]:SER:HB2	1.98	0.63
1:C:44[A]:THR:HG23	3:C:4752[A]:FAD:PA	2.38	0.63
1:E:195[A]:SER:O	1:E:199[A]:ARG:HG3	1.98	0.63
1:F:44[A]:THR:CG2	3:F:4755[A]:FAD:PA	2.80	0.63
3:B:4752[C]:FAD:PA	1:C:44[C]:THR:HG23	2.38	0.63
1:E:195[C]:SER:O	1:E:199[C]:ARG:HG3	1.98	0.63
3:E:4755[C]:FAD:PA	1:F:44[C]:THR:CG2	2.80	0.63
1:C:52[A]:PRO:HG3	1:C:96[A]:VAL:HG21	1.80	0.63
4:C:4801[A]:HOH:O	1:D:427[A]:GLU:HG3	1.98	0.63
1:F:17[A]:GLY:O	1:F:21[A]:ALA:HB2	1.99	0.63
1:G:430[A]:ASN:HD21	1:H:451[A]:ALA:H	1.46	0.63
1:I:208[A]:GLU:HB3	1:I:239[A]:LEU:HD23	1.80	0.63
4:B:4801[C]:HOH:O	1:D:427[C]:GLU:HG3	1.98	0.63
1:C:52[C]:PRO:HG3	1:C:96[C]:VAL:HG21	1.80	0.63
1:F:17[C]:GLY:O	1:F:21[C]:ALA:HB2	1.99	0.63
1:G:430[C]:ASN:HD21	1:H:451[C]:ALA:H	1.46	0.63
1:I:208[C]:GLU:HB3	1:I:239[C]:LEU:HD23	1.80	0.63
1:B:380[A]:GLU:CG	1:J:84[A]:ASN:ND2	2.62	0.63
2:L:132[A]:SER:O	2:L:135[A]:ALA:N	2.31	0.63
1:B:380[C]:GLU:CG	1:J:84[C]:ASN:ND2	2.62	0.63
1:A:96[A]:VAL:O	1:A:100[A]:THR:HG23	1.97	0.63
1:E:305[A]:ASN:ND2	1:E:305[A]:ASN:C	2.50	0.63
1:I:33[A]:VAL:HA	1:I:113[A]:VAL:HG23	1.80	0.63
1:A:96[C]:VAL:O	1:A:100[C]:THR:HG23	1.97	0.63
1:E:305[C]:ASN:ND2	1:E:305[C]:ASN:C	2.50	0.63
1:G:348[C]:HIS:CE1	2:N:136[C]:ARG:CD	2.70	0.63
1:I:33[C]:VAL:HA	1:I:113[C]:VAL:HG23	1.80	0.63
1:B:60[A]:SER:HB2	1:B:200[A]:LEU:CD1	2.28	0.63
1:E:443[A]:GLU:O	1:E:447[A]:ARG:HB2	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:222[A]:ILE:HG13	1:H:223[A]:SER:H	1.63	0.63
1:I:57[A]:LEU:HD23	1:I:196[A]:VAL:HG22	1.80	0.63
1:B:60[C]:SER:HB2	1:B:200[C]:LEU:CD1	2.28	0.63
1:E:443[C]:GLU:O	1:E:447[C]:ARG:HB2	1.98	0.63
1:H:222[C]:ILE:HG13	1:H:223[C]:SER:H	1.63	0.63
1:I:57[C]:LEU:HD23	1:I:196[C]:VAL:HG22	1.80	0.63
1:G:239[A]:LEU:H	1:G:239[A]:LEU:HD12	1.62	0.62
1:G:239[C]:LEU:H	1:G:239[C]:LEU:HD12	1.62	0.62
2:N:134[C]:ALA:O	2:N:138[C]:ILE:HG13	1.98	0.62
1:A:278[A]:ILE:O	1:A:278[A]:ILE:HG12	1.98	0.62
1:B:142[A]:LYS:HE3	4:H:4814[A]:HOH:O	1.99	0.62
1:C:242[A]:LYS:HD3	1:C:259[A]:GLU:HG2	1.80	0.62
1:E:116[A]:ASN:HD22	1:E:117[A]:GLY:N	1.97	0.62
1:J:122[A]:THR:HG23	1:J:128[A]:THR:CG2	2.29	0.62
1:A:278[C]:ILE:O	1:A:278[C]:ILE:HG12	1.98	0.62
1:B:142[C]:LYS:HE3	4:G:4814[C]:HOH:O	1.99	0.62
1:C:242[C]:LYS:HD3	1:C:259[C]:GLU:HG2	1.80	0.62
1:E:116[C]:ASN:HD22	1:E:117[C]:GLY:N	1.97	0.62
1:J:122[C]:THR:HG23	1:J:128[C]:THR:CG2	2.29	0.62
1:H:258[A]:ILE:O	1:H:259[A]:GLU:HB2	1.99	0.62
1:J:135[A]:GLY:O	1:J:136[A]:THR:O	2.16	0.62
2:M:142[A]:HIS:CD2	2:M:167[A]:VAL:HG13	2.33	0.62
1:H:258[C]:ILE:O	1:H:259[C]:GLU:HB2	1.99	0.62
1:J:135[C]:GLY:O	1:J:136[C]:THR:O	2.16	0.62
1:A:46[A]:LEU:HD23	1:A:103[A]:ILE:CD1	2.28	0.62
1:C:409[A]:GLN:HG2	1:C:412[A]:THR:OG1	1.98	0.62
1:F:84[A]:ASN:HD21	1:F:86[A]:ASP:HB2	1.64	0.62
3:I:4758[A]:FAD:O4'	3:I:4758[A]:FAD:O2'	2.16	0.62
1:A:46[C]:LEU:HD23	1:A:103[C]:ILE:CD1	2.28	0.62
1:C:409[C]:GLN:HG2	1:C:412[C]:THR:OG1	1.98	0.62
1:F:84[C]:ASN:HD21	1:F:86[C]:ASP:HB2	1.64	0.62
2:N:155[C]:ARG:O	2:N:157[C]:ILE:N	2.32	0.62
1:B:431[A]:GLU:OE2	1:B:450[A]:HIS:CE1	2.51	0.62
1:C:3[A]:GLN:HE21	1:C:3[A]:GLN:CA	2.10	0.62
1:E:81[A]:VAL:HG22	1:F:78[A]:MET:HG2	1.81	0.62
1:H:265[A]:LYS:NZ	1:H:265[A]:LYS:CB	2.63	0.62
1:I:11[A]:VAL:HG13	1:I:145[A]:LEU:CD2	2.24	0.62
1:J:17[A]:GLY:H	1:J:20[A]:VAL:CG2	2.12	0.62
1:B:431[C]:GLU:OE2	1:B:450[C]:HIS:CE1	2.51	0.62
1:C:3[C]:GLN:HE21	1:C:3[C]:GLN:CA	2.10	0.62
1:E:81[C]:VAL:HG22	1:F:78[C]:MET:HG2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:265[C]:LYS:NZ	1:H:265[C]:LYS:CB	2.63	0.62
1:I:11[C]:VAL:HG13	1:I:145[C]:LEU:CD2	2.24	0.62
1:J:17[C]:GLY:H	1:J:20[C]:VAL:CG2	2.12	0.62
1:C:448[A]:VAL:HG21	1:D:434[A]:LEU:HD12	1.81	0.62
1:D:333[A]:ASP:O	1:D:337[A]:ILE:HG12	1.99	0.62
1:I:296[A]:LEU:O	1:I:297[A]:ASP:C	2.36	0.62
1:C:448[C]:VAL:HG21	1:D:434[C]:LEU:HD12	1.81	0.62
1:D:333[C]:ASP:O	1:D:337[C]:ILE:HG12	1.99	0.62
1:I:296[C]:LEU:O	1:I:297[C]:ASP:C	2.36	0.62
1:G:189[A]:ILE:H	1:G:189[A]:ILE:HD13	1.62	0.62
1:G:189[C]:ILE:HD13	1:G:189[C]:ILE:H	1.62	0.62
2:L:167[C]:VAL:O	2:L:171[C]:GLN:HB3	2.00	0.62
1:H:265[A]:LYS:HB2	1:H:265[A]:LYS:NZ	2.13	0.62
1:I:184[A]:ILE:CG2	1:I:278[A]:ILE:HD11	2.29	0.62
1:J:209[A]:PHE:CD1	1:J:209[A]:PHE:O	2.53	0.62
1:H:265[C]:LYS:HB2	1:H:265[C]:LYS:NZ	2.13	0.62
1:I:184[C]:ILE:CG2	1:I:278[C]:ILE:HD11	2.29	0.62
1:J:209[C]:PHE:O	1:J:209[C]:PHE:CD1	2.53	0.62
1:E:78[A]:MET:H	1:E:78[A]:MET:HE2	1.62	0.62
2:M:144[A]:LEU:HD21	2:M:170[A]:LYS:HE3	1.82	0.62
1:E:78[C]:MET:H	1:E:78[C]:MET:HE2	1.62	0.62
1:A:51[A]:ILE:HB	1:A:52[A]:PRO:HD3	1.82	0.62
1:A:137[A]:GLN:HE21	1:A:137[A]:GLN:CA	2.13	0.62
1:A:351[A]:TYR:O	1:A:354[A]:VAL:HG12	2.00	0.62
1:H:392[A]:SER:O	1:H:396[A]:THR:HG23	2.00	0.62
1:J:439[A]:GLY:O	1:J:440[A]:ALA:O	2.17	0.62
1:A:51[C]:ILE:HB	1:A:52[C]:PRO:HD3	1.82	0.62
1:A:137[C]:GLN:HE21	1:A:137[C]:GLN:CA	2.13	0.62
1:A:351[C]:TYR:O	1:A:354[C]:VAL:HG12	2.00	0.62
1:H:392[C]:SER:O	1:H:396[C]:THR:HG23	2.00	0.62
1:J:439[C]:GLY:O	1:J:440[C]:ALA:O	2.17	0.62
2:N:131[C]:LEU:CD2	2:N:146[C]:ALA:CB	2.74	0.62
2:L:157[A]:ILE:HG22	2:L:158[A]:PHE:N	2.15	0.61
1:H:438[C]:TYR:CD1	2:N:157[C]:ILE:HD11	2.34	0.61
1:D:144[A]:ILE:HG23	1:D:315[A]:ILE:HG12	1.82	0.61
1:D:410[A]:LYS:HG3	1:D:410[A]:LYS:O	2.00	0.61
1:D:420[A]:ILE:HG12	1:D:428[A]:MET:HE2	1.81	0.61
1:J:244[A]:THR:OG1	1:J:257[A]:SER:HB3	1.99	0.61
1:D:144[C]:ILE:HG23	1:D:315[C]:ILE:HG12	1.82	0.61
1:D:410[C]:LYS:HG3	1:D:410[C]:LYS:O	2.00	0.61
1:D:420[C]:ILE:HG12	1:D:428[C]:MET:HE2	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:244[C]:THR:OG1	1:J:257[C]:SER:HB3	1.99	0.61
1:C:7[A]:ALA:O	1:C:141[A]:THR:HA	2.00	0.61
1:C:137[A]:GLN:CA	1:C:137[A]:GLN:NE2	2.62	0.61
1:D:44[A]:THR:CG2	3:D:4753[A]:FAD:O2A	2.47	0.61
1:E:209[A]:PHE:HA	1:E:241[A]:THR:O	2.00	0.61
1:C:7[C]:ALA:O	1:C:141[C]:THR:HA	2.00	0.61
1:C:137[C]:GLN:CA	1:C:137[C]:GLN:NE2	2.62	0.61
3:C:4753[C]:FAD:O2A	1:D:44[C]:THR:CG2	2.47	0.61
1:E:209[C]:PHE:HA	1:E:241[C]:THR:O	2.00	0.61
1:G:139[A]:ILE:HD12	1:G:139[A]:ILE:N	2.14	0.61
1:I:244[A]:THR:HB	1:I:257[A]:SER:HB3	1.82	0.61
1:J:308[A]:PHE:O	1:J:316[A]:TYR:HB3	2.01	0.61
2:K:152[A]:THR:O	2:K:153[A]:GLY:O	2.17	0.61
1:G:139[C]:ILE:HD12	1:G:139[C]:ILE:N	2.14	0.61
1:I:244[C]:THR:HB	1:I:257[C]:SER:HB3	1.82	0.61
1:J:308[C]:PHE:O	1:J:316[C]:TYR:HB3	2.01	0.61
1:D:69[A]:LYS:O	1:D:69[A]:LYS:CG	2.48	0.61
1:F:51[A]:ILE:HB	1:F:52[A]:PRO:HD3	1.83	0.61
1:F:162[A]:GLU:OE1	1:F:162[A]:GLU:HA	2.00	0.61
1:D:69[C]:LYS:O	1:D:69[C]:LYS:CG	2.48	0.61
1:F:51[C]:ILE:HB	1:F:52[C]:PRO:HD3	1.83	0.61
1:F:162[C]:GLU:OE1	1:F:162[C]:GLU:HA	2.00	0.61
1:A:215[A]:GLY:HA3	4:A:4762[A]:HOH:O	2.00	0.61
1:A:442[A]:CYS:HB2	1:A:467[A]:SER:HB3	1.82	0.61
1:C:249[A]:LYS:HD3	1:C:255[A]:ASP:OD2	2.00	0.61
1:E:93[A]:SER:O	1:E:97[A]:LYS:HD3	2.00	0.61
1:G:209[A]:PHE:O	1:G:240[A]:ASN:HA	2.00	0.61
2:O:131[A]:LEU:HD21	2:O:135[A]:ALA:HB3	1.82	0.61
1:A:215[C]:GLY:HA3	4:J:4762[C]:HOH:O	2.00	0.61
1:A:442[C]:CYS:HB2	1:A:467[C]:SER:HB3	1.82	0.61
1:C:249[C]:LYS:HD3	1:C:255[C]:ASP:OD2	2.00	0.61
1:E:93[C]:SER:O	1:E:97[C]:LYS:HD3	2.00	0.61
1:G:209[C]:PHE:O	1:G:240[C]:ASN:HA	2.00	0.61
1:C:299[A]:ARG:HD3	1:C:301[A]:ARG:NH2	2.16	0.61
3:C:4752[A]:FAD:O4'	3:C:4752[A]:FAD:O2'	2.16	0.61
3:B:4752[C]:FAD:O2'	3:B:4752[C]:FAD:O4'	2.16	0.61
1:C:299[C]:ARG:HD3	1:C:301[C]:ARG:NH2	2.16	0.61
2:N:158[C]:PHE:CE2	2:N:163[C]:ALA:HA	2.33	0.61
1:A:84[A]:ASN:C	1:A:84[A]:ASN:HD22	2.04	0.61
1:G:51[A]:ILE:HG23	1:H:396[A]:THR:CG2	2.30	0.61
1:G:358[A]:ILE:CG2	1:G:364[A]:VAL:HB	2.27	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:397[A]:ASN:N	1:H:397[A]:ASN:ND2	2.47	0.61
2:N:131[A]:LEU:CD2	2:N:136[A]:ARG:HA	2.30	0.61
1:A:84[C]:ASN:HD22	1:A:84[C]:ASN:C	2.04	0.61
1:G:51[C]:ILE:HG23	1:H:396[C]:THR:CG2	2.30	0.61
1:G:358[C]:ILE:CG2	1:G:364[C]:VAL:HB	2.27	0.61
1:H:397[C]:ASN:N	1:H:397[C]:ASN:ND2	2.47	0.61
1:C:347[A]:VAL:HG23	1:C:347[A]:VAL:O	1.99	0.61
1:C:442[A]:CYS:HA	1:C:463[A]:ASN:HD22	1.65	0.61
1:C:347[C]:VAL:HG23	1:C:347[C]:VAL:O	1.99	0.61
1:C:442[C]:CYS:HA	1:C:463[C]:ASN:HD22	1.65	0.61
1:A:248[A]:LYS:NZ	1:A:248[A]:LYS:CB	2.63	0.61
1:D:12[A]:ILE:CD1	1:D:144[A]:ILE:HD11	2.30	0.61
1:H:54[A]:LYS:HD3	1:H:54[A]:LYS:N	2.14	0.61
1:I:36[A]:GLU:OE2	1:I:38[A]:ASN:HB2	2.01	0.61
1:I:189[A]:ILE:HG23	3:I:4758[A]:FAD:HM73	1.82	0.61
1:I:464[A]:LEU:HD23	1:I:470[A]:LYS:O	2.01	0.61
1:J:50[A]:CYS:O	1:J:54[A]:LYS:HE2	1.99	0.61
1:A:248[C]:LYS:NZ	1:A:248[C]:LYS:CB	2.63	0.61
1:B:45[C]:CYS:SG	1:B:50[C]:CYS:SG	2.85	0.61
1:D:12[C]:ILE:CD1	1:D:144[C]:ILE:HD11	2.30	0.61
1:H:54[C]:LYS:HD3	1:H:54[C]:LYS:N	2.14	0.61
3:H:4758[C]:FAD:HM73	1:I:189[C]:ILE:HG23	1.82	0.61
1:I:36[C]:GLU:OE2	1:I:38[C]:ASN:HB2	2.01	0.61
1:I:464[C]:LEU:HD23	1:I:470[C]:LYS:O	2.01	0.61
1:J:50[C]:CYS:O	1:J:54[C]:LYS:HE2	1.99	0.61
1:A:455[A]:LEU:HD22	1:A:455[A]:LEU:N	2.16	0.60
1:D:431[A]:GLU:OE2	1:D:450[A]:HIS:HE1	1.84	0.60
1:G:158[A]:ILE:CD1	1:G:246[A]:ALA:HB3	2.31	0.60
1:G:358[A]:ILE:HD13	1:G:360[A]:THR:H	1.65	0.60
1:H:5[A]:ILE:HG23	1:H:137[A]:GLN:NE2	2.16	0.60
1:H:267[A]:GLU:HG2	1:H:268[A]:VAL:H	1.66	0.60
1:H:330[A]:LYS:HD3	1:H:334[A]:GLU:CD	2.21	0.60
1:I:7[A]:ALA:HB1	1:I:31[A]:LYS:O	2.00	0.60
1:A:455[C]:LEU:HD22	1:A:455[C]:LEU:N	2.16	0.60
1:D:431[C]:GLU:OE2	1:D:450[C]:HIS:HE1	1.84	0.60
1:G:158[C]:ILE:CD1	1:G:246[C]:ALA:HB3	2.31	0.60
1:G:358[C]:ILE:HD13	1:G:360[C]:THR:H	1.65	0.60
1:H:5[C]:ILE:HG23	1:H:137[C]:GLN:NE2	2.16	0.60
1:H:267[C]:GLU:HG2	1:H:268[C]:VAL:H	1.66	0.60
1:H:330[C]:LYS:HD3	1:H:334[C]:GLU:CD	2.21	0.60
1:I:7[C]:ALA:HB1	1:I:31[C]:LYS:O	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330[A]:LYS:O	1:A:334[A]:GLU:HG3	2.01	0.60
1:A:428[A]:MET:HE1	1:A:455[A]:LEU:HB3	1.81	0.60
1:E:409[A]:GLN:CG	1:E:412[A]:THR:HG23	2.32	0.60
1:H:414[A]:ARG:HH11	1:H:414[A]:ARG:CG	2.14	0.60
2:O:131[A]:LEU:HD23	2:O:132[A]:SER:N	2.16	0.60
2:O:138[A]:ILE:O	2:O:141[A]:LYS:N	2.25	0.60
1:A:330[C]:LYS:O	1:A:334[C]:GLU:HG3	2.01	0.60
1:A:428[C]:MET:HE1	1:A:455[C]:LEU:HB3	1.81	0.60
1:E:409[C]:GLN:CG	1:E:412[C]:THR:HG23	2.32	0.60
1:H:414[C]:ARG:HH11	1:H:414[C]:ARG:CG	2.14	0.60
1:A:46[A]:LEU:HD23	1:A:103[A]:ILE:HD11	1.81	0.60
1:B:180[A]:LYS:HB2	1:B:180[A]:LYS:HZ3	1.65	0.60
1:D:165[A]:ILE:HD11	1:D:254[A]:ILE:HG12	1.81	0.60
1:I:380[A]:GLU:HG2	1:I:410[A]:LYS:HG3	1.83	0.60
2:N:130[A]:ARG:O	2:N:158[A]:PHE:N	2.34	0.60
2:N:168[A]:GLN:O	2:N:171[A]:GLN:N	2.32	0.60
1:A:46[C]:LEU:HD23	1:A:103[C]:ILE:HD11	1.81	0.60
1:B:180[C]:LYS:HB2	1:B:180[C]:LYS:HZ3	1.65	0.60
1:D:165[C]:ILE:HD11	1:D:254[C]:ILE:HG12	1.81	0.60
1:I:380[C]:GLU:HG2	1:I:410[C]:LYS:HG3	1.83	0.60
1:C:320[A]:ASP:CG	1:C:326[A]:MET:HG2	2.22	0.60
1:C:375[A]:LYS:HE3	1:C:381[A]:TYR:OH	2.01	0.60
1:J:294[A]:ILE:HG21	1:J:310[A]:THR:HB	1.82	0.60
1:J:305[A]:ASN:HD21	1:J:309[A]:GLN:HG3	1.64	0.60
2:K:131[A]:LEU:HD23	2:K:136[A]:ARG:HB2	1.83	0.60
2:O:145[A]:ASP:HB3	2:O:148[A]:GLN:HG2	1.82	0.60
1:C:320[C]:ASP:CG	1:C:326[C]:MET:HG2	2.22	0.60
1:C:375[C]:LYS:HE3	1:C:381[C]:TYR:OH	2.01	0.60
1:J:294[C]:ILE:HG21	1:J:310[C]:THR:HB	1.82	0.60
1:J:305[C]:ASN:HD21	1:J:309[C]:GLN:HG3	1.64	0.60
1:A:334[A]:GLU:OE2	1:A:351[A]:TYR:OH	2.17	0.60
1:J:46[A]:LEU:HD12	1:J:46[A]:LEU:O	2.02	0.60
1:A:334[C]:GLU:OE2	1:A:351[C]:TYR:OH	2.17	0.60
1:J:46[C]:LEU:HD12	1:J:46[C]:LEU:O	2.02	0.60
1:A:304[A]:VAL:HG23	1:F:250[A]:SER:HB3	1.83	0.60
1:D:191[A]:VAL:O	1:D:195[A]:SER:HB2	2.02	0.60
1:E:46[A]:LEU:HD11	1:E:99[A]:LEU:HB3	1.82	0.60
1:H:121[A]:ILE:HG12	1:H:144[A]:ILE:CD1	2.32	0.60
1:A:304[C]:VAL:HG23	1:F:250[C]:SER:HB3	1.83	0.60
1:D:191[C]:VAL:O	1:D:195[C]:SER:HB2	2.02	0.60
1:E:46[C]:LEU:HD11	1:E:99[C]:LEU:HB3	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:121[C]:ILE:HG12	1:H:144[C]:ILE:CD1	2.32	0.60
1:A:16[A]:PRO:O	1:A:20[A]:VAL:HG13	2.02	0.60
1:A:23[A]:ILE:O	1:A:27[A]:GLN:HG3	2.01	0.60
1:G:125[A]:ASN:HD22	1:G:142[A]:LYS:HA	1.65	0.60
1:G:248[A]:LYS:H	1:G:248[A]:LYS:HD2	1.66	0.60
1:J:305[A]:ASN:H	1:J:305[A]:ASN:HD22	1.46	0.60
1:A:16[C]:PRO:O	1:A:20[C]:VAL:HG13	2.02	0.60
1:A:23[C]:ILE:O	1:A:27[C]:GLN:HG3	2.01	0.60
1:E:45[C]:CYS:SG	1:E:50[C]:CYS:SG	2.62	0.60
1:G:125[C]:ASN:HD22	1:G:142[C]:LYS:HA	1.65	0.60
1:G:248[C]:LYS:H	1:G:248[C]:LYS:HD2	1.66	0.60
1:J:305[C]:ASN:H	1:J:305[C]:ASN:HD22	1.46	0.60
2:L:138[C]:ILE:HD12	2:L:164[C]:LEU:HD23	1.82	0.60
1:E:297[A]:ASP:HB2	1:E:298[A]:PRO:HD2	1.83	0.60
1:F:44[A]:THR:HG21	3:F:4755[A]:FAD:O2A	1.99	0.60
1:J:301[A]:ARG:NH1	1:J:323[A]:ALA:HA	2.16	0.60
1:E:297[C]:ASP:HB2	1:E:298[C]:PRO:HD2	1.83	0.60
3:E:4755[C]:FAD:O2A	1:F:44[C]:THR:HG21	1.99	0.60
1:J:301[C]:ARG:NH1	1:J:323[C]:ALA:HA	2.16	0.60
1:C:414[A]:ARG:CG	1:C:414[A]:ARG:NH1	2.52	0.60
1:F:116[A]:ASN:C	1:F:116[A]:ASN:HD22	2.04	0.60
1:H:41[A]:LEU:HD13	1:H:103[A]:ILE:HG22	1.84	0.60
1:H:220[A]:MET:CE	1:H:220[A]:MET:CB	2.80	0.60
1:H:453[A]:PRO:HA	1:H:457[A]:GLU:OE1	2.02	0.60
1:I:9[A]:VAL:CG2	1:I:342[A]:MET:HE1	2.31	0.60
1:J:122[A]:THR:CG2	1:J:128[A]:THR:HG21	2.31	0.60
1:C:414[C]:ARG:CG	1:C:414[C]:ARG:NH1	2.52	0.60
1:F:116[C]:ASN:C	1:F:116[C]:ASN:HD22	2.04	0.60
1:H:41[C]:LEU:HD13	1:H:103[C]:ILE:HG22	1.84	0.60
1:H:220[C]:MET:CE	1:H:220[C]:MET:CB	2.80	0.60
1:H:453[C]:PRO:HA	1:H:457[C]:GLU:OE1	2.02	0.60
1:I:9[C]:VAL:CG2	1:I:342[C]:MET:HE1	2.31	0.60
1:J:122[C]:THR:CG2	1:J:128[C]:THR:HG21	2.31	0.60
2:N:133[C]:PRO:HA	2:N:136[C]:ARG:HH21	1.66	0.60
1:A:209[A]:PHE:O	1:A:240[A]:ASN:HA	2.02	0.60
1:A:451[A]:ALA:O	1:A:454[A]:THR:HG23	2.01	0.60
1:D:133[A]:ASP:CG	1:D:133[A]:ASP:O	2.40	0.60
1:D:255[A]:ASP:OD1	1:D:270[A]:THR:HB	2.01	0.60
1:E:180[A]:LYS:HD3	1:E:203[A]:ASP:O	2.02	0.60
1:H:83[A]:LEU:HD13	1:H:84[A]:ASN:H	1.67	0.60
1:H:162[A]:GLU:HA	1:H:162[A]:GLU:OE1	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:155[A]:PHE:CZ	1:I:243[A]:VAL:HG23	2.37	0.60
1:I:387[A]:PRO:HA	1:I:403[A]:MET:HB3	1.83	0.60
1:I:388[A]:PHE:CE2	1:I:422[A]:GLY:HA3	2.36	0.60
2:N:164[A]:LEU:O	2:N:167[A]:VAL:N	2.35	0.60
1:A:209[C]:PHE:O	1:A:240[C]:ASN:HA	2.02	0.60
1:A:451[C]:ALA:O	1:A:454[C]:THR:HG23	2.01	0.60
1:D:133[C]:ASP:CG	1:D:133[C]:ASP:O	2.40	0.60
1:D:255[C]:ASP:OD1	1:D:270[C]:THR:HB	2.01	0.60
1:E:180[C]:LYS:HD3	1:E:203[C]:ASP:O	2.02	0.60
1:H:83[C]:LEU:HD13	1:H:84[C]:ASN:H	1.67	0.60
1:H:162[C]:GLU:OE1	1:H:162[C]:GLU:HA	2.01	0.60
1:I:155[C]:PHE:CZ	1:I:243[C]:VAL:HG23	2.37	0.60
1:I:387[C]:PRO:HA	1:I:403[C]:MET:HB3	1.83	0.60
1:I:388[C]:PHE:CE2	1:I:422[C]:GLY:HA3	2.36	0.60
2:N:131[C]:LEU:HD21	2:N:146[C]:ALA:HB1	1.81	0.60
1:B:337[A]:ILE:HG13	1:B:347[A]:VAL:HG13	1.84	0.59
1:D:89[A]:MET:HE3	1:D:92[A]:LYS:HE2	1.83	0.59
1:G:150[A]:SER:HB3	1:G:320[A]:ASP:OD2	2.02	0.59
1:G:299[A]:ARG:HH11	1:G:299[A]:ARG:HG3	1.67	0.59
1:I:218[A]:ILE:N	1:I:218[A]:ILE:CD1	2.53	0.59
1:B:337[C]:ILE:HG13	1:B:347[C]:VAL:HG13	1.84	0.59
1:D:89[C]:MET:HE3	1:D:92[C]:LYS:HE2	1.83	0.59
1:G:150[C]:SER:HB3	1:G:320[C]:ASP:OD2	2.02	0.59
1:G:299[C]:ARG:HG3	1:G:299[C]:ARG:HH11	1.67	0.59
1:I:218[C]:ILE:N	1:I:218[C]:ILE:CD1	2.53	0.59
1:G:178[A]:PRO:HB3	1:G:273[A]:VAL:CG2	2.31	0.59
1:H:370[A]:SER:H	1:H:373[A]:GLN:NE2	2.00	0.59
1:I:307[A]:ARG:NH1	1:I:347[A]:VAL:HG22	2.17	0.59
1:I:381[A]:TYR:CD1	1:I:381[A]:TYR:C	2.76	0.59
2:M:142[A]:HIS:CD2	2:M:167[A]:VAL:CG1	2.85	0.59
1:G:178[C]:PRO:HB3	1:G:273[C]:VAL:CG2	2.31	0.59
1:H:370[C]:SER:H	1:H:373[C]:GLN:NE2	2.00	0.59
1:I:307[C]:ARG:NH1	1:I:347[C]:VAL:HG22	2.17	0.59
1:I:381[C]:TYR:C	1:I:381[C]:TYR:CD1	2.76	0.59
1:A:105[A]:HIS:HD2	4:A:4772[A]:HOH:O	1.86	0.59
1:I:372[A]:GLU:C	1:I:374[A]:LEU:H	2.04	0.59
1:A:105[C]:HIS:HD2	4:J:4772[C]:HOH:O	1.86	0.59
1:I:372[C]:GLU:C	1:I:374[C]:LEU:H	2.04	0.59
2:N:159[C]:THR:CG2	2:N:161[C]:GLU:H	2.16	0.59
1:B:304[A]:VAL:HG23	1:J:250[A]:SER:HB3	1.84	0.59
1:G:239[A]:LEU:O	1:G:240[A]:ASN:HB2	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:314[A]:ASN:H	1:G:314[A]:ASN:ND2	1.97	0.59
1:I:244[A]:THR:HB	1:I:257[A]:SER:CB	2.32	0.59
1:J:325[A]:PRO:O	1:J:330[A]:LYS:HD2	2.02	0.59
1:B:304[C]:VAL:HG23	1:J:250[C]:SER:HB3	1.84	0.59
1:G:239[C]:LEU:O	1:G:240[C]:ASN:HB2	2.02	0.59
1:G:314[C]:ASN:H	1:G:314[C]:ASN:ND2	1.97	0.59
1:I:244[C]:THR:HB	1:I:257[C]:SER:CB	2.32	0.59
1:J:325[C]:PRO:O	1:J:330[C]:LYS:HD2	2.02	0.59
1:H:155[A]:PHE:HD2	1:H:278[A]:ILE:HD11	1.68	0.59
1:J:209[A]:PHE:CD1	1:J:209[A]:PHE:C	2.76	0.59
1:H:155[C]:PHE:HD2	1:H:278[C]:ILE:HD11	1.68	0.59
1:J:209[C]:PHE:CD1	1:J:209[C]:PHE:C	2.76	0.59
2:M:153[C]:GLY:O	2:M:154[C]:PRO:O	2.21	0.59
1:J:37[A]:LYS:HG2	4:J:4759[A]:FAD:N3A	2.16	0.59
2:L:172[A]:THR:O	2:L:173[A]:GLY:C	2.39	0.59
3:I:4759[C]:FAD:N3A	1:J:37[C]:LYS:HG2	2.16	0.59
1:A:434[A]:LEU:HD12	1:B:448[A]:VAL:HG21	1.85	0.59
1:B:305[A]:ASN:C	1:B:305[A]:ASN:HD22	2.06	0.59
1:D:187[A]:GLY:O	1:D:191[A]:VAL:CG2	2.51	0.59
3:F:4755[A]:FAD:C4X	4:F:4797[A]:HOH:O	2.51	0.59
1:A:434[C]:LEU:HD12	1:B:448[C]:VAL:HG21	1.85	0.59
1:B:305[C]:ASN:HD22	1:B:305[C]:ASN:C	2.06	0.59
1:D:187[C]:GLY:O	1:D:191[C]:VAL:CG2	2.51	0.59
3:E:4755[C]:FAD:C4X	4:E:4797[C]:HOH:O	2.51	0.59
2:K:167[A]:VAL:O	2:K:171[A]:GLN:NE2	2.35	0.59
2:M:142[A]:HIS:HD2	2:M:167[A]:VAL:CG1	2.15	0.59
1:F:6[A]:ASP:O	1:F:31[A]:LYS:HE3	2.02	0.59
1:F:6[C]:ASP:O	1:F:31[C]:LYS:HE3	2.02	0.59
1:C:434[A]:LEU:O	1:C:434[A]:LEU:HD23	2.03	0.59
1:G:314[A]:ASN:HD22	1:G:314[A]:ASN:N	1.95	0.59
1:A:441[C]:SER:HB3	2:K:155[C]:ARG:HH22	1.68	0.59
1:C:434[C]:LEU:O	1:C:434[C]:LEU:HD23	2.03	0.59
1:G:314[C]:ASN:HD22	1:G:314[C]:ASN:N	1.95	0.59
2:K:134[C]:ALA:O	2:K:137[C]:ASN:HB3	2.03	0.59
1:E:409[A]:GLN:NE2	1:E:411[A]:SER:N	2.40	0.58
1:I:297[A]:ASP:C	1:I:299[A]:ARG:N	2.56	0.58
2:M:135[A]:ALA:HA	2:M:138[A]:ILE:CD1	2.32	0.58
1:E:409[C]:GLN:NE2	1:E:411[C]:SER:N	2.40	0.58
1:I:297[C]:ASP:C	1:I:299[C]:ARG:N	2.56	0.58
2:M:146[C]:ALA:O	2:M:149[C]:GLY:N	2.26	0.58
1:D:284[A]:THR:HG22	1:D:284[A]:THR:O	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:188[A]:VAL:HG22	1:F:358[A]:ILE:HG12	1.86	0.58
1:G:10[A]:THR:OG1	1:G:141[A]:THR:HG21	2.04	0.58
1:G:171[A]:ALA:HB3	1:G:193[A]:LEU:HD23	1.83	0.58
1:G:203[A]:ASP:OD1	1:G:236[A]:LYS:HE2	2.03	0.58
2:L:172[A]:THR:O	2:L:172[A]:THR:HG22	2.01	0.58
1:D:284[C]:THR:O	1:D:284[C]:THR:HG22	2.02	0.58
1:F:188[C]:VAL:HG22	1:F:358[C]:ILE:HG12	1.86	0.58
1:G:10[C]:THR:OG1	1:G:141[C]:THR:HG21	2.04	0.58
1:G:171[C]:ALA:HB3	1:G:193[C]:LEU:HD23	1.83	0.58
1:G:203[C]:ASP:OD1	1:G:236[C]:LYS:HE2	2.03	0.58
1:D:338[A]:CYS:O	1:D:342[A]:MET:HG3	2.03	0.58
1:J:8[A]:ASP:HB2	1:J:142[A]:LYS:HG3	1.85	0.58
2:L:131[A]:LEU:O	2:L:157[A]:ILE:CG2	2.52	0.58
2:N:155[A]:ARG:HG2	2:N:156[A]:GLY:H	1.68	0.58
1:D:338[C]:CYS:O	1:D:342[C]:MET:HG3	2.03	0.58
1:J:8[C]:ASP:HB2	1:J:142[C]:LYS:HG3	1.85	0.58
1:E:137[A]:GLN:NE2	1:E:138[A]:VAL:N	2.51	0.58
1:F:435[A]:ALA:HB1	1:F:445[A]:ILE:HD11	1.84	0.58
1:J:122[A]:THR:HG23	1:J:128[A]:THR:HG22	1.84	0.58
2:M:155[A]:ARG:HH21	2:M:157[A]:ILE:HG22	1.68	0.58
2:M:159[A]:THR:CG2	2:M:161[A]:GLU:HB2	2.33	0.58
1:E:137[C]:GLN:NE2	1:E:138[C]:VAL:N	2.51	0.58
1:F:435[C]:ALA:HB1	1:F:445[C]:ILE:HD11	1.84	0.58
1:J:122[C]:THR:HG23	1:J:128[C]:THR:HG22	1.84	0.58
1:C:413[A]:ASP:O	1:C:441[A]:SER:HB2	2.03	0.58
1:E:361[A]:HIS:HE1	1:E:399[A]:ASP:OD2	1.87	0.58
1:G:155[A]:PHE:CZ	1:G:243[A]:VAL:HG13	2.39	0.58
1:I:155[A]:PHE:CZ	1:I:243[A]:VAL:CG2	2.86	0.58
1:C:413[C]:ASP:O	1:C:441[C]:SER:HB2	2.03	0.58
1:E:361[C]:HIS:HE1	1:E:399[C]:ASP:OD2	1.87	0.58
1:G:155[C]:PHE:CZ	1:G:243[C]:VAL:HG13	2.39	0.58
1:I:155[C]:PHE:CZ	1:I:243[C]:VAL:CG2	2.86	0.58
1:E:347[A]:VAL:HG23	1:E:347[A]:VAL:O	2.03	0.58
1:F:16[A]:PRO:O	1:F:18[A]:GLY:N	2.37	0.58
1:E:347[C]:VAL:O	1:E:347[C]:VAL:HG23	2.03	0.58
1:F:16[C]:PRO:O	1:F:18[C]:GLY:N	2.37	0.58
1:D:450[A]:HIS:CD2	1:D:460[A]:ARG:HG3	2.38	0.58
1:E:434[A]:LEU:HD23	1:F:434[A]:LEU:HD23	1.86	0.58
1:G:248[A]:LYS:HD2	1:G:248[A]:LYS:N	2.19	0.58
1:D:450[C]:HIS:CD2	1:D:460[C]:ARG:HG3	2.38	0.58
1:E:434[C]:LEU:HD23	1:F:434[C]:LEU:HD23	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:248[C]:LYS:HD2	1:G:248[C]:LYS:N	2.19	0.58
2:M:141[C]:LYS:CD	2:M:141[C]:LYS:C	2.72	0.58
1:B:60[A]:SER:HB2	1:B:200[A]:LEU:HD13	1.84	0.58
1:D:284[A]:THR:HB	4:D:4772[A]:HOH:O	2.04	0.58
1:G:74[A]:ARG:HE	1:H:59[A]:ASN:ND2	2.01	0.58
1:I:320[A]:ASP:OD2	3:I:4758[A]:FAD:H5'1	2.04	0.58
1:B:60[C]:SER:HB2	1:B:200[C]:LEU:HD13	1.84	0.58
4:C:4772[C]:HOH:O	1:D:284[C]:THR:HB	2.04	0.58
1:G:74[C]:ARG:HE	1:H:59[C]:ASN:ND2	2.01	0.58
3:H:4758[C]:FAD:H5'1	1:I:320[C]:ASP:OD2	2.04	0.58
2:K:159[C]:THR:HG22	2:K:161[C]:GLU:H	1.68	0.58
1:E:219[A]:ASP:HB3	1:E:222[A]:ILE:HG23	1.86	0.58
1:E:219[C]:ASP:HB3	1:E:222[C]:ILE:HG23	1.86	0.58
1:A:173[A]:SER:O	1:A:174[A]:LEU:C	2.41	0.58
1:A:174[A]:LEU:HB2	1:A:197[A]:TRP:CZ2	2.38	0.58
1:C:307[A]:ARG:O	1:C:308[A]:PHE:HB2	2.04	0.58
1:C:363[A]:GLU:HB2	1:C:425[A]:ALA:HB3	1.86	0.58
1:D:193[A]:LEU:N	1:D:193[A]:LEU:CD1	2.66	0.58
1:I:336[A]:ILE:CG2	1:I:337[A]:ILE:N	2.67	0.58
2:K:171[A]:GLN:O	2:K:172[A]:THR:C	2.39	0.58
1:A:173[C]:SER:O	1:A:174[C]:LEU:C	2.41	0.58
1:A:174[C]:LEU:HB2	1:A:197[C]:TRP:CZ2	2.38	0.58
1:C:307[C]:ARG:O	1:C:308[C]:PHE:HB2	2.04	0.58
1:C:363[C]:GLU:HB2	1:C:425[C]:ALA:HB3	1.86	0.58
1:D:193[C]:LEU:N	1:D:193[C]:LEU:CD1	2.66	0.58
1:I:336[C]:ILE:CG2	1:I:337[C]:ILE:N	2.67	0.58
1:B:145[A]:LEU:HD11	1:B:318[A]:ILE:HD12	1.86	0.57
1:I:78[A]:MET:SD	1:J:78[A]:MET:HE3	2.43	0.57
2:K:137[A]:ASN:HD22	2:K:137[A]:ASN:C	2.07	0.57
1:B:145[C]:LEU:HD11	1:B:318[C]:ILE:HD12	1.86	0.57
1:I:78[C]:MET:SD	1:J:78[C]:MET:HE3	2.43	0.57
2:L:138[C]:ILE:HD11	2:L:167[C]:VAL:HG21	1.86	0.57
1:C:3[A]:GLN:HA	1:C:3[A]:GLN:NE2	2.18	0.57
1:C:46[A]:LEU:CD2	1:C:100[A]:THR:HG22	2.35	0.57
1:D:406[A]:ILE:HD13	1:D:463[A]:ASN:CG	2.23	0.57
1:I:336[A]:ILE:HG22	1:I:337[A]:ILE:N	2.18	0.57
1:J:384[A]:GLY:O	1:J:406[A]:ILE:CD1	2.52	0.57
2:M:131[A]:LEU:CD1	2:M:136[A]:ARG:NH2	2.67	0.57
2:M:132[A]:SER:O	2:M:135[A]:ALA:N	2.37	0.57
1:C:3[C]:GLN:HA	1:C:3[C]:GLN:NE2	2.18	0.57
1:C:46[C]:LEU:CD2	1:C:100[C]:THR:HG22	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:406[C]:ILE:HD13	1:D:463[C]:ASN:CG	2.23	0.57
1:I:336[C]:ILE:HG22	1:I:337[C]:ILE:N	2.18	0.57
1:J:384[C]:GLY:O	1:J:406[C]:ILE:CD1	2.52	0.57
2:M:134[C]:ALA:O	2:M:138[C]:ILE:HG13	2.04	0.57
1:D:51[A]:ILE:HB	1:D:52[A]:PRO:CD	2.29	0.57
1:I:9[A]:VAL:HG22	1:I:342[A]:MET:HE1	1.87	0.57
1:I:160[A]:ILE:HA	1:I:165[A]:ILE:HG22	1.86	0.57
4:J:4759[A]:FAD:O4'	4:J:4759[A]:FAD:O2'	2.16	0.57
1:D:51[C]:ILE:HB	1:D:52[C]:PRO:CD	2.29	0.57
1:I:9[C]:VAL:HG22	1:I:342[C]:MET:HE1	1.87	0.57
1:I:160[C]:ILE:HA	1:I:165[C]:ILE:HG22	1.86	0.57
3:I:4759[C]:FAD:O4'	3:I:4759[C]:FAD:O2'	2.16	0.57
1:C:393[A]:ARG:HB3	1:C:455[A]:LEU:HD13	1.86	0.57
1:G:178[A]:PRO:HB3	1:G:273[A]:VAL:HG23	1.85	0.57
1:C:393[C]:ARG:HB3	1:C:455[C]:LEU:HD13	1.86	0.57
1:G:178[C]:PRO:HB3	1:G:273[C]:VAL:HG23	1.85	0.57
1:A:354[A]:VAL:HG13	1:A:354[A]:VAL:O	2.04	0.57
1:D:301[A]:ARG:NH1	1:D:323[A]:ALA:HA	2.19	0.57
1:I:441[A]:SER:O	1:I:444[A]:ASP:HB2	2.05	0.57
1:J:434[A]:LEU:O	1:J:434[A]:LEU:HD12	2.05	0.57
2:K:137[A]:ASN:C	2:K:137[A]:ASN:ND2	2.58	0.57
2:M:170[A]:LYS:C	2:M:170[A]:LYS:HD3	2.25	0.57
1:A:354[C]:VAL:HG13	1:A:354[C]:VAL:O	2.04	0.57
1:D:301[C]:ARG:NH1	1:D:323[C]:ALA:HA	2.19	0.57
1:I:441[C]:SER:O	1:I:444[C]:ASP:HB2	2.05	0.57
1:J:434[C]:LEU:HD12	1:J:434[C]:LEU:O	2.05	0.57
1:C:46[A]:LEU:HD23	1:C:100[A]:THR:HG22	1.86	0.57
1:D:330[A]:LYS:CE	1:D:334[A]:GLU:OE2	2.50	0.57
1:J:25[A]:ALA:HB2	1:J:339[A]:VAL:HG11	1.86	0.57
1:J:413[A]:ASP:O	1:J:441[A]:SER:HB2	2.04	0.57
1:C:46[C]:LEU:HD23	1:C:100[C]:THR:HG22	1.86	0.57
1:D:330[C]:LYS:CE	1:D:334[C]:GLU:OE2	2.50	0.57
1:J:25[C]:ALA:HB2	1:J:339[C]:VAL:HG11	1.86	0.57
1:J:413[C]:ASP:O	1:J:441[C]:SER:HB2	2.04	0.57
2:L:138[C]:ILE:HD11	2:L:167[C]:VAL:CG2	2.35	0.57
1:C:31[A]:LYS:NZ	4:C:4765[A]:HOH:O	2.37	0.57
1:C:208[A]:GLU:HB3	1:C:239[A]:LEU:HD12	1.86	0.57
1:I:291[A]:GLU:O	1:I:292[A]:LEU:HD12	2.05	0.57
1:I:435[A]:ALA:CB	1:I:445[A]:ILE:HD11	2.34	0.57
1:J:345[A]:GLY:HA2	2:O:141[A]:LYS:HD3	1.85	0.57
4:B:4765[C]:HOH:O	1:C:31[C]:LYS:NZ	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:208[C]:GLU:HB3	1:C:239[C]:LEU:HD12	1.86	0.57
1:I:291[C]:GLU:O	1:I:292[C]:LEU:HD12	2.05	0.57
1:I:435[C]:ALA:CB	1:I:445[C]:ILE:HD11	2.34	0.57
1:A:69[A]:LYS:HB2	1:A:69[A]:LYS:NZ	2.20	0.57
1:B:429[A]:VAL:O	1:B:432[A]:ALA:HB3	2.05	0.57
1:E:204[A]:VAL:HG12	1:E:205[A]:THR:N	2.19	0.57
1:J:37[A]:LYS:HE3	4:J:4759[A]:FAD:C5A	2.35	0.57
2:O:152[A]:THR:HB	2:O:162[A]:ASP:OD1	2.05	0.57
1:A:69[C]:LYS:HB2	1:A:69[C]:LYS:NZ	2.20	0.57
1:A:441[C]:SER:N	2:K:155[C]:ARG:NH2	2.53	0.57
1:B:429[C]:VAL:O	1:B:432[C]:ALA:HB3	2.05	0.57
1:E:204[C]:VAL:HG12	1:E:205[C]:THR:N	2.19	0.57
3:I:4759[C]:FAD:C5A	1:J:37[C]:LYS:HE3	2.35	0.57
1:G:70[A]:ASP:OD1	1:G:74[A]:ARG:NH1	2.37	0.57
1:G:322[A]:VAL:CG1	1:G:323[A]:ALA:N	2.68	0.57
1:H:172[A]:LEU:HD13	1:H:193[A]:LEU:HD11	1.86	0.57
1:J:232[A]:LYS:N	1:J:232[A]:LYS:HE3	2.20	0.57
1:G:70[C]:ASP:OD1	1:G:74[C]:ARG:NH1	2.37	0.57
1:G:322[C]:VAL:CG1	1:G:323[C]:ALA:N	2.68	0.57
1:H:172[C]:LEU:HD13	1:H:193[C]:LEU:HD11	1.86	0.57
1:J:232[C]:LYS:N	1:J:232[C]:LYS:HE3	2.20	0.57
1:A:430[A]:ASN:ND2	1:B:450[A]:HIS:HA	2.20	0.56
1:B:45[A]:CYS:HG	1:B:50[A]:CYS:CB	2.16	0.56
1:H:428[A]:MET:HE1	1:H:455[A]:LEU:HB3	1.86	0.56
1:H:461[A]:GLU:OE2	1:H:473[A]:ASN:OD1	2.22	0.56
2:M:152[A]:THR:H	2:M:162[A]:ASP:CG	2.08	0.56
1:A:430[C]:ASN:ND2	1:B:450[C]:HIS:HA	2.20	0.56
1:B:45[C]:CYS:HG	1:B:50[C]:CYS:CB	2.16	0.56
1:H:428[C]:MET:HE1	1:H:455[C]:LEU:HB3	1.86	0.56
1:H:461[C]:GLU:OE2	1:H:473[C]:ASN:OD1	2.22	0.56
1:E:453[A]:PRO:HA	1:E:457[A]:GLU:OE2	2.04	0.56
1:H:377[A]:GLU:HG3	1:H:379[A]:ILE:HD12	1.87	0.56
1:I:155[A]:PHE:HD2	1:I:158[A]:ILE:HG13	1.70	0.56
1:J:406[A]:ILE:HG21	1:J:463[A]:ASN:ND2	2.20	0.56
2:M:132[A]:SER:O	2:M:133[A]:PRO:C	2.43	0.56
1:E:453[C]:PRO:HA	1:E:457[C]:GLU:OE2	2.04	0.56
1:H:377[C]:GLU:HG3	1:H:379[C]:ILE:HD12	1.87	0.56
1:I:155[C]:PHE:HD2	1:I:158[C]:ILE:HG13	1.70	0.56
1:J:406[C]:ILE:HG21	1:J:463[C]:ASN:ND2	2.20	0.56
1:B:188[A]:VAL:HG22	1:B:358[A]:ILE:HG12	1.87	0.56
1:C:88[A]:MET:CE	1:C:200[A]:LEU:HD21	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:161[A]:ASP:OD1	1:D:163[A]:ASP:HB3	2.06	0.56
1:E:41[A]:LEU:CD1	1:E:103[A]:ILE:HG22	2.35	0.56
1:E:204[A]:VAL:CG1	1:E:205[A]:THR:N	2.68	0.56
1:F:320[A]:ASP:HA	4:F:4765[A]:HOH:O	2.03	0.56
1:F:438[A]:TYR:CD1	2:M:133[A]:PRO:HD2	2.39	0.56
1:G:137[A]:GLN:NE2	1:G:138[A]:VAL:H	1.97	0.56
1:H:165[A]:ILE:HG23	1:H:274[A]:LEU:HD23	1.87	0.56
1:I:63[A]:TYR:HA	1:J:76[A]:ILE:HD13	1.87	0.56
1:I:76[A]:ILE:HD13	1:J:63[A]:TYR:CA	2.35	0.56
1:J:305[A]:ASN:ND2	1:J:309[A]:GLN:H	2.03	0.56
2:L:170[A]:LYS:O	2:L:170[A]:LYS:HD3	2.04	0.56
2:N:133[A]:PRO:O	2:N:136[A]:ARG:HG2	2.05	0.56
2:N:158[A]:PHE:CE1	2:N:162[A]:ASP:HB3	2.41	0.56
1:B:188[C]:VAL:HG22	1:B:358[C]:ILE:HG12	1.87	0.56
1:C:88[C]:MET:CE	1:C:200[C]:LEU:HD21	2.35	0.56
1:D:161[C]:ASP:OD1	1:D:163[C]:ASP:HB3	2.06	0.56
1:E:41[C]:LEU:CD1	1:E:103[C]:ILE:HG22	2.35	0.56
1:E:204[C]:VAL:CG1	1:E:205[C]:THR:N	2.68	0.56
4:E:4765[C]:HOH:O	1:F:320[C]:ASP:HA	2.03	0.56
1:G:137[C]:GLN:NE2	1:G:138[C]:VAL:H	1.97	0.56
1:H:165[C]:ILE:HG23	1:H:274[C]:LEU:HD23	1.87	0.56
1:I:63[C]:TYR:HA	1:J:76[C]:ILE:HD13	1.87	0.56
1:I:76[C]:ILE:HD13	1:J:63[C]:TYR:CA	2.35	0.56
1:J:305[C]:ASN:ND2	1:J:309[C]:GLN:H	2.03	0.56
1:B:137[A]:GLN:CA	1:B:137[A]:GLN:NE2	2.64	0.56
1:B:275[A]:LEU:CD2	1:B:275[A]:LEU:C	2.74	0.56
1:B:318[A]:ILE:HG12	1:B:319[A]:GLY:N	2.19	0.56
2:K:142[A]:HIS:O	2:K:143[A]:SER:C	2.44	0.56
2:N:146[A]:ALA:O	2:N:148[A]:GLN:N	2.38	0.56
1:B:137[C]:GLN:CA	1:B:137[C]:GLN:NE2	2.64	0.56
1:B:275[C]:LEU:C	1:B:275[C]:LEU:CD2	2.74	0.56
1:B:318[C]:ILE:HG12	1:B:319[C]:GLY:N	2.19	0.56
1:E:137[A]:GLN:HE21	1:E:137[A]:GLN:HA	1.67	0.56
1:H:56[A]:LEU:HD12	1:H:172[A]:LEU:HD12	1.86	0.56
1:H:428[A]:MET:CE	1:H:455[A]:LEU:HB3	2.35	0.56
1:I:289[A]:LEU:HD12	1:I:289[A]:LEU:H	1.69	0.56
1:E:137[C]:GLN:HE21	1:E:137[C]:GLN:HA	1.67	0.56
1:H:56[C]:LEU:HD12	1:H:172[C]:LEU:HD12	1.86	0.56
1:H:428[C]:MET:CE	1:H:455[C]:LEU:HB3	2.35	0.56
1:I:289[C]:LEU:HD12	1:I:289[C]:LEU:H	1.69	0.56
2:M:142[C]:HIS:O	2:M:144[C]:LEU:HG	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:454[A]:THR:HB	1:D:427[A]:GLU:OE1	2.06	0.56
1:D:14[A]:SER:O	1:D:19[A]:TYR:HB3	2.05	0.56
1:I:376[A]:GLU:C	1:I:378[A]:GLY:H	2.08	0.56
1:I:434[A]:LEU:HD13	1:J:448[A]:VAL:HG21	1.87	0.56
2:N:148[A]:GLN:HG3	2:N:148[A]:GLN:O	2.06	0.56
1:C:454[C]:THR:HB	1:D:427[C]:GLU:OE1	2.06	0.56
1:D:14[C]:SER:O	1:D:19[C]:TYR:HB3	2.05	0.56
1:D:443[C]:GLU:OE2	2:L:134[C]:ALA:HB1	2.06	0.56
1:H:45[C]:CYS:SG	1:H:50[C]:CYS:SG	2.98	0.56
1:I:376[C]:GLU:C	1:I:378[C]:GLY:H	2.08	0.56
1:I:434[C]:LEU:HD13	1:J:448[C]:VAL:HG21	1.87	0.56
1:G:413[A]:ASP:HB3	2:N:160[A]:LYS:HE2	1.87	0.56
1:A:316[A]:TYR:N	1:A:316[A]:TYR:CD1	2.72	0.56
1:A:358[A]:ILE:HD11	1:A:360[A]:THR:OG1	2.06	0.56
1:E:116[A]:ASN:HD22	1:E:116[A]:ASN:C	2.09	0.56
1:F:440[A]:ALA:HA	2:M:155[A]:ARG:NH1	2.20	0.56
1:J:56[A]:LEU:HD21	1:J:92[A]:LYS:HD3	1.87	0.56
1:A:316[C]:TYR:N	1:A:316[C]:TYR:CD1	2.72	0.56
1:A:358[C]:ILE:HD11	1:A:360[C]:THR:OG1	2.06	0.56
1:E:116[C]:ASN:HD22	1:E:116[C]:ASN:C	2.09	0.56
1:F:412[C]:THR:HB	2:M:161[C]:GLU:HG2	1.87	0.56
1:J:56[C]:LEU:HD21	1:J:92[C]:LYS:HD3	1.87	0.56
1:F:453[A]:PRO:HA	1:F:457[A]:GLU:OE2	2.06	0.56
1:I:65[A]:MET:CE	1:I:71[A]:PHE:HE1	2.19	0.56
1:J:51[A]:ILE:CB	1:J:52[A]:PRO:HD3	2.27	0.56
1:A:441[C]:SER:N	2:K:155[C]:ARG:HH21	2.04	0.56
1:F:453[C]:PRO:HA	1:F:457[C]:GLU:OE2	2.06	0.56
1:I:65[C]:MET:CE	1:I:71[C]:PHE:HE1	2.19	0.56
1:J:51[C]:ILE:CB	1:J:52[C]:PRO:HD3	2.27	0.56
1:F:188[A]:VAL:CG2	1:F:358[A]:ILE:HG12	2.36	0.56
1:G:330[A]:LYS:HD3	1:G:334[A]:GLU:OE2	2.06	0.56
1:I:44[A]:THR:HG23	3:I:4758[A]:FAD:O2A	2.05	0.56
2:O:131[A]:LEU:HD21	2:O:135[A]:ALA:CB	2.36	0.56
1:F:188[C]:VAL:CG2	1:F:358[C]:ILE:HG12	2.36	0.56
1:G:330[C]:LYS:HD3	1:G:334[C]:GLU:OE2	2.06	0.56
3:H:4758[C]:FAD:O2A	1:I:44[C]:THR:HG23	2.05	0.56
1:D:43[A]:GLY:HA2	3:D:4753[A]:FAD:O3B	2.06	0.55
1:E:412[A]:THR:O	1:E:413[A]:ASP:HB3	2.07	0.55
1:E:461[A]:GLU:OE2	1:E:472[A]:ILE:HG22	2.06	0.55
1:F:461[A]:GLU:OE2	1:F:473[A]:ASN:ND2	2.38	0.55
1:G:443[A]:GLU:O	1:G:447[A]:ARG:HG3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:152[A]:THR:O	2:M:162[A]:ASP:OD2	2.24	0.55
3:C:4753[C]:FAD:O3B	1:D:43[C]:GLY:HA2	2.06	0.55
1:E:412[C]:THR:O	1:E:413[C]:ASP:HB3	2.07	0.55
1:E:461[C]:GLU:OE2	1:E:472[C]:ILE:HG22	2.06	0.55
1:F:461[C]:GLU:OE2	1:F:473[C]:ASN:ND2	2.38	0.55
1:G:443[C]:GLU:O	1:G:447[C]:ARG:HG3	2.06	0.55
1:B:355[A]:PRO:HA	1:B:367[A]:VAL:HG23	1.88	0.55
1:F:318[A]:ILE:HB	1:F:334[A]:GLU:HB3	1.87	0.55
1:H:305[A]:ASN:ND2	1:H:307[A]:ARG:N	2.54	0.55
1:I:15[A]:GLY:N	4:I:4760[A]:HOH:O	2.38	0.55
1:I:301[A]:ARG:HD2	1:I:323[A]:ALA:HA	1.89	0.55
2:M:152[A]:THR:CG2	2:M:153[A]:GLY:N	2.68	0.55
2:M:168[A]:GLN:O	2:M:171[A]:GLN:HG3	2.05	0.55
1:B:355[C]:PRO:HA	1:B:367[C]:VAL:HG23	1.88	0.55
1:F:318[C]:ILE:HB	1:F:334[C]:GLU:HB3	1.87	0.55
1:G:45[C]:CYS:SG	1:G:50[C]:CYS:SG	2.71	0.55
1:H:305[C]:ASN:ND2	1:H:307[C]:ARG:N	2.54	0.55
4:H:4760[C]:HOH:O	1:I:15[C]:GLY:N	2.38	0.55
1:I:301[C]:ARG:HD2	1:I:323[C]:ALA:HA	1.89	0.55
1:A:443[A]:GLU:HB2	2:K:160[A]:LYS:NZ	2.21	0.55
1:D:7[A]:ALA:O	1:D:141[A]:THR:HA	2.06	0.55
1:E:160[A]:ILE:HA	1:E:165[A]:ILE:HG22	1.89	0.55
1:I:80[A]:GLU:HG2	1:I:81[A]:VAL:N	2.22	0.55
1:D:7[C]:ALA:O	1:D:141[C]:THR:HA	2.06	0.55
1:E:160[C]:ILE:HA	1:E:165[C]:ILE:HG22	1.89	0.55
1:I:80[C]:GLU:HG2	1:I:81[C]:VAL:N	2.22	0.55
1:A:186[A]:ALA:HB1	1:A:213[A]:VAL:HG13	1.88	0.55
1:E:116[A]:ASN:C	1:E:116[A]:ASN:ND2	2.58	0.55
1:G:404[A]:VAL:HG22	1:G:420[A]:ILE:HG23	1.89	0.55
1:H:165[A]:ILE:CD1	1:H:254[A]:ILE:HD12	2.36	0.55
1:H:318[A]:ILE:HD12	1:H:335[A]:GLY:CA	2.35	0.55
1:I:92[A]:LYS:O	1:I:96[A]:VAL:HG23	2.06	0.55
1:I:320[A]:ASP:HB3	1:I:326[A]:MET:CE	2.37	0.55
1:A:186[C]:ALA:HB1	1:A:213[C]:VAL:HG13	1.88	0.55
1:E:116[C]:ASN:C	1:E:116[C]:ASN:ND2	2.58	0.55
1:G:404[C]:VAL:HG22	1:G:420[C]:ILE:HG23	1.89	0.55
1:H:165[C]:ILE:CD1	1:H:254[C]:ILE:HD12	2.36	0.55
1:H:318[C]:ILE:HD12	1:H:335[C]:GLY:CA	2.35	0.55
1:I:92[C]:LYS:O	1:I:96[C]:VAL:HG23	2.06	0.55
1:I:320[C]:ASP:HB3	1:I:326[C]:MET:CE	2.37	0.55
1:D:87[A]:LYS:HE3	1:D:90[A]:GLU:OE1	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:25[A]:ALA:HB3	1:E:32[A]:THR:HG21	1.88	0.55
1:F:184[A]:ILE:HG22	1:F:278[A]:ILE:CG2	2.37	0.55
1:G:10[A]:THR:HG23	1:G:33[A]:VAL:HG22	1.89	0.55
1:H:275[A]:LEU:HD12	1:H:276[A]:VAL:N	2.21	0.55
1:D:87[C]:LYS:HE3	1:D:90[C]:GLU:OE1	2.05	0.55
1:E:25[C]:ALA:HB3	1:E:32[C]:THR:HG21	1.88	0.55
1:F:184[C]:ILE:HG22	1:F:278[C]:ILE:CG2	2.37	0.55
1:G:10[C]:THR:HG23	1:G:33[C]:VAL:HG22	1.89	0.55
1:H:275[C]:LEU:HD12	1:H:276[C]:VAL:N	2.21	0.55
1:G:27[A]:GLN:HE21	1:G:110[A]:ASN:HD21	1.53	0.55
1:H:44[A]:THR:HG23	3:H:4757[A]:FAD:O2A	2.07	0.55
1:H:258[A]:ILE:HD13	1:H:269[A]:ILE:HD11	1.88	0.55
1:I:9[A]:VAL:HG22	1:I:143[A]:ASN:HB2	1.87	0.55
2:L:139[A]:LEU:O	2:L:142[A]:HIS:N	2.36	0.55
1:G:27[C]:GLN:HE21	1:G:110[C]:ASN:HD21	1.53	0.55
3:G:4757[C]:FAD:O2A	1:H:44[C]:THR:HG23	2.07	0.55
1:H:258[C]:ILE:HD13	1:H:269[C]:ILE:HD11	1.88	0.55
1:I:9[C]:VAL:HG22	1:I:143[C]:ASN:HB2	1.87	0.55
1:B:82[A]:ARG:HH11	1:B:82[A]:ARG:HG3	1.70	0.55
1:H:449[A]:CYS:HA	1:H:460[A]:ARG:NH2	2.22	0.55
1:I:284[A]:THR:O	1:I:285[A]:LYS:C	2.44	0.55
1:B:82[C]:ARG:HG3	1:B:82[C]:ARG:HH11	1.70	0.55
1:H:449[C]:CYS:HA	1:H:460[C]:ARG:NH2	2.22	0.55
1:I:284[C]:THR:O	1:I:285[C]:LYS:C	2.44	0.55
1:F:143[A]:ASN:CB	1:F:342[A]:MET:HE1	2.37	0.55
1:G:57[A]:LEU:HD23	1:G:196[A]:VAL:HG23	1.88	0.55
1:G:305[A]:ASN:OD1	1:G:305[A]:ASN:C	2.45	0.55
1:J:255[A]:ASP:OD1	1:J:270[A]:THR:HB	2.07	0.55
2:L:151[A]:ALA:HB1	2:L:158[A]:PHE:HA	1.85	0.55
1:F:143[C]:ASN:CB	1:F:342[C]:MET:HE1	2.37	0.55
1:G:57[C]:LEU:HD23	1:G:196[C]:VAL:HG23	1.88	0.55
1:G:305[C]:ASN:C	1:G:305[C]:ASN:OD1	2.45	0.55
1:J:255[C]:ASP:OD1	1:J:270[C]:THR:HB	2.07	0.55
1:B:144[A]:ILE:HD12	1:B:144[A]:ILE:C	2.28	0.55
1:C:43[A]:GLY:O	1:C:47[A]:ASN:HB2	2.07	0.55
1:E:320[A]:ASP:OD2	3:E:4754[A]:FAD:H5'1	2.06	0.55
1:F:412[A]:THR:O	1:F:413[A]:ASP:HB3	2.06	0.55
1:G:3[A]:GLN:CB	1:G:4[A]:PRO:HD2	2.36	0.55
1:G:84[A]:ASN:C	1:G:84[A]:ASN:ND2	2.60	0.55
1:G:158[A]:ILE:HD11	1:G:246[A]:ALA:HB3	1.89	0.55
1:H:431[A]:GLU:OE2	1:H:450[A]:HIS:CE1	2.57	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:383[A]:VAL:HG23	1:I:407[A]:LEU:CD2	2.36	0.55
1:I:396[A]:THR:O	1:I:398[A]:ALA:N	2.40	0.55
2:L:166[A]:LEU:O	2:L:167[A]:VAL:C	2.44	0.55
2:M:131[A]:LEU:HD11	2:M:136[A]:ARG:NH2	2.22	0.55
1:B:144[C]:ILE:HD12	1:B:144[C]:ILE:C	2.28	0.55
1:C:43[C]:GLY:O	1:C:47[C]:ASN:HB2	2.07	0.55
3:D:4754[C]:FAD:H5'1	1:E:320[C]:ASP:OD2	2.06	0.55
1:F:412[C]:THR:O	1:F:413[C]:ASP:HB3	2.06	0.55
1:G:3[C]:GLN:CB	1:G:4[C]:PRO:HD2	2.36	0.55
1:G:84[C]:ASN:C	1:G:84[C]:ASN:ND2	2.60	0.55
1:G:158[C]:ILE:HD11	1:G:246[C]:ALA:HB3	1.89	0.55
1:H:431[C]:GLU:OE2	1:H:450[C]:HIS:CE1	2.57	0.55
1:I:383[C]:VAL:HG23	1:I:407[C]:LEU:CD2	2.36	0.55
1:I:396[C]:THR:O	1:I:398[C]:ALA:N	2.40	0.55
1:A:198[A]:GLN:HB2	1:A:204[A]:VAL:HG21	1.89	0.55
1:E:137[A]:GLN:NE2	1:E:137[A]:GLN:HA	2.21	0.55
1:F:146[A]:ILE:CG2	1:F:148[A]:THR:HG23	2.37	0.55
1:A:198[C]:GLN:HB2	1:A:204[C]:VAL:HG21	1.89	0.55
1:E:137[C]:GLN:NE2	1:E:137[C]:GLN:HA	2.21	0.55
1:F:146[C]:ILE:CG2	1:F:148[C]:THR:HG23	2.37	0.55
2:M:159[C]:THR:CG2	2:M:162[C]:ASP:N	2.61	0.55
1:A:46[A]:LEU:CD2	1:A:103[A]:ILE:HD11	2.37	0.54
1:C:3[A]:GLN:CG	1:C:4[A]:PRO:HD2	2.31	0.54
1:E:131[A]:LYS:NZ	1:E:132[A]:ALA:H	2.04	0.54
1:G:254[A]:ILE:HD12	1:G:255[A]:ASP:N	2.21	0.54
1:H:10[A]:THR:HG23	1:H:141[A]:THR:CB	2.36	0.54
1:A:46[C]:LEU:CD2	1:A:103[C]:ILE:HD11	2.37	0.54
1:C:3[C]:GLN:CG	1:C:4[C]:PRO:HD2	2.31	0.54
1:E:131[C]:LYS:NZ	1:E:132[C]:ALA:H	2.04	0.54
1:G:254[C]:ILE:HD12	1:G:255[C]:ASP:N	2.21	0.54
1:H:10[C]:THR:HG23	1:H:141[C]:THR:CB	2.36	0.54
2:L:142[C]:HIS:O	2:L:144[C]:LEU:CD2	2.55	0.54
2:N:157[C]:ILE:HG22	2:N:158[C]:PHE:N	2.22	0.54
1:A:182[A]:VAL:CG2	1:A:274[A]:LEU:HD13	2.37	0.54
1:B:44[A]:THR:HG23	3:B:4751[A]:FAD:O2A	2.07	0.54
1:C:259[A]:GLU:HA	1:C:265[A]:LYS:O	2.07	0.54
1:D:165[A]:ILE:CD1	1:D:254[A]:ILE:HG12	2.38	0.54
1:E:41[A]:LEU:HD13	1:E:103[A]:ILE:HG22	1.87	0.54
1:G:442[A]:CYS:CA	1:G:463[A]:ASN:HD22	2.15	0.54
1:H:184[A]:ILE:HD11	1:H:274[A]:LEU:HD11	1.88	0.54
1:I:456[A]:SER:HB2	1:J:430[A]:ASN:OD1	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182[C]:VAL:CG2	1:A:274[C]:LEU:HD13	2.37	0.54
3:A:4751[C]:FAD:O2A	1:B:44[C]:THR:HG23	2.07	0.54
1:C:259[C]:GLU:HA	1:C:265[C]:LYS:O	2.07	0.54
1:D:165[C]:ILE:CD1	1:D:254[C]:ILE:HG12	2.38	0.54
1:E:41[C]:LEU:HD13	1:E:103[C]:ILE:HG22	1.87	0.54
1:G:442[C]:CYS:CA	1:G:463[C]:ASN:HD22	2.15	0.54
1:H:184[C]:ILE:HD11	1:H:274[C]:LEU:HD11	1.88	0.54
1:I:456[C]:SER:HB2	1:J:430[C]:ASN:OD1	2.08	0.54
2:M:172[C]:THR:CG2	2:M:172[C]:THR:CA	2.76	0.54
2:N:159[C]:THR:HG22	2:N:161[C]:GLU:CA	2.37	0.54
1:B:412[A]:THR:O	1:B:414[A]:ARG:N	2.40	0.54
1:D:12[A]:ILE:HD12	1:D:144[A]:ILE:HD11	1.88	0.54
1:G:358[A]:ILE:HD13	1:G:358[A]:ILE:O	2.07	0.54
1:H:267[A]:GLU:HG2	1:H:268[A]:VAL:N	2.22	0.54
1:I:265[A]:LYS:O	1:I:266[A]:ALA:O	2.25	0.54
1:I:391[A]:ASN:HB3	1:I:394[A]:ALA:HB3	1.90	0.54
1:J:225[A]:ASN:OD1	1:J:403[A]:MET:CE	2.55	0.54
1:J:227[A]:GLN:O	1:J:231[A]:GLN:HG3	2.07	0.54
1:J:365[A]:ALA:HB3	1:J:425[A]:ALA:O	2.08	0.54
1:B:412[C]:THR:O	1:B:414[C]:ARG:N	2.40	0.54
1:D:12[C]:ILE:HD12	1:D:144[C]:ILE:HD11	1.88	0.54
1:G:358[C]:ILE:HD13	1:G:358[C]:ILE:O	2.07	0.54
1:H:267[C]:GLU:HG2	1:H:268[C]:VAL:N	2.22	0.54
1:I:265[C]:LYS:O	1:I:266[C]:ALA:O	2.25	0.54
1:I:391[C]:ASN:HB3	1:I:394[C]:ALA:HB3	1.90	0.54
1:J:225[C]:ASN:OD1	1:J:403[C]:MET:CE	2.55	0.54
1:J:227[C]:GLN:O	1:J:231[C]:GLN:HG3	2.07	0.54
1:J:365[C]:ALA:HB3	1:J:425[C]:ALA:O	2.08	0.54
1:A:74[A]:ARG:HH21	1:B:59[A]:ASN:HD21	1.55	0.54
1:E:46[A]:LEU:HD23	1:E:100[A]:THR:HG22	1.87	0.54
1:E:220[A]:MET:CE	1:E:220[A]:MET:CG	2.85	0.54
1:F:139[A]:ILE:HD12	1:F:139[A]:ILE:N	2.23	0.54
1:F:256[A]:VAL:CG2	1:F:269[A]:ILE:HB	2.36	0.54
1:H:121[A]:ILE:HG12	1:H:144[A]:ILE:HD11	1.89	0.54
1:J:263[A]:GLY:HA3	1:J:265[A]:LYS:NZ	2.22	0.54
2:K:171[A]:GLN:CD	2:K:171[A]:GLN:N	2.58	0.54
1:A:74[C]:ARG:HH21	1:B:59[C]:ASN:HD21	1.55	0.54
1:E:46[C]:LEU:HD23	1:E:100[C]:THR:HG22	1.87	0.54
1:E:220[C]:MET:CE	1:E:220[C]:MET:CG	2.85	0.54
1:F:139[C]:ILE:HD12	1:F:139[C]:ILE:N	2.23	0.54
1:F:256[C]:VAL:CG2	1:F:269[C]:ILE:HB	2.36	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:121[C]:ILE:HG12	1:H:144[C]:ILE:HD11	1.89	0.54
1:J:263[C]:GLY:HA3	1:J:265[C]:LYS:NZ	2.22	0.54
1:E:305[A]:ASN:ND2	1:E:307[A]:ARG:H	2.05	0.54
1:E:396[A]:THR:HG21	1:F:54[A]:LYS:HB3	1.90	0.54
1:H:10[A]:THR:HG21	1:H:139[A]:ILE:CG2	2.37	0.54
1:E:305[C]:ASN:ND2	1:E:307[C]:ARG:H	2.05	0.54
1:E:396[C]:THR:HG21	1:F:54[C]:LYS:HB3	1.90	0.54
1:E:440[C]:ALA:HA	2:M:155[C]:ARG:HH12	1.73	0.54
1:H:10[C]:THR:HG21	1:H:139[C]:ILE:CG2	2.37	0.54
1:A:46[A]:LEU:HD12	1:A:46[A]:LEU:C	2.28	0.54
1:D:318[A]:ILE:HB	1:D:334[A]:GLU:HB3	1.90	0.54
1:E:312[A]:ILE:HD11	1:E:314[A]:ASN:ND2	2.22	0.54
1:G:386[A]:PHE:O	1:G:403[A]:MET:HB2	2.07	0.54
2:K:150[A]:THR:O	2:K:162[A]:ASP:OD2	2.25	0.54
1:A:46[C]:LEU:HD12	1:A:46[C]:LEU:C	2.28	0.54
1:D:318[C]:ILE:HB	1:D:334[C]:GLU:HB3	1.90	0.54
1:E:312[C]:ILE:HD11	1:E:314[C]:ASN:ND2	2.22	0.54
1:G:386[C]:PHE:O	1:G:403[C]:MET:HB2	2.07	0.54
1:A:213[A]:VAL:HG12	1:A:214[A]:GLY:N	2.22	0.54
1:E:150[A]:SER:OG	1:E:280[A]:ARG:NH1	2.41	0.54
1:F:291[A]:GLU:OE1	1:F:291[A]:GLU:N	2.41	0.54
1:I:123[A]:GLY:O	1:I:125[A]:ASN:N	2.40	0.54
1:J:327[A]:LEU:HD13	1:J:329[A]:HIS:CE1	2.43	0.54
2:K:171[A]:GLN:C	2:K:173[A]:GLY:N	2.61	0.54
2:L:139[A]:LEU:O	2:L:140[A]:GLU:C	2.46	0.54
2:L:151[A]:ALA:HB1	2:L:157[A]:ILE:O	2.08	0.54
1:A:213[C]:VAL:HG12	1:A:214[C]:GLY:N	2.22	0.54
1:E:150[C]:SER:OG	1:E:280[C]:ARG:NH1	2.41	0.54
1:F:291[C]:GLU:OE1	1:F:291[C]:GLU:N	2.41	0.54
1:I:123[C]:GLY:O	1:I:125[C]:ASN:N	2.40	0.54
1:J:327[C]:LEU:HD13	1:J:329[C]:HIS:CE1	2.43	0.54
2:K:167[C]:VAL:HG13	2:K:171[C]:GLN:OE1	2.07	0.54
1:A:182[A]:VAL:HG23	1:A:274[A]:LEU:HD13	1.90	0.54
1:D:305[A]:ASN:H	1:D:305[A]:ASN:HD22	1.54	0.54
1:J:413[A]:ASP:OD2	1:J:442[A]:CYS:HB2	2.08	0.54
1:A:182[C]:VAL:HG23	1:A:274[C]:LEU:HD13	1.90	0.54
1:D:305[C]:ASN:HD22	1:D:305[C]:ASN:H	1.54	0.54
1:J:413[C]:ASP:OD2	1:J:442[C]:CYS:HB2	2.08	0.54
1:C:262[A]:SER:O	1:C:263[A]:GLY:O	2.26	0.54
1:E:191[A]:VAL:O	1:E:195[A]:SER:HB2	2.08	0.54
1:I:150[A]:SER:OG	1:I:280[A]:ARG:NH1	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:160[A]:ILE:HD11	1:J:276[A]:VAL:HB	1.90	0.54
1:C:262[C]:SER:O	1:C:263[C]:GLY:O	2.26	0.54
1:E:191[C]:VAL:O	1:E:195[C]:SER:HB2	2.08	0.54
1:I:150[C]:SER:OG	1:I:280[C]:ARG:NH1	2.41	0.54
1:J:160[C]:ILE:HD11	1:J:276[C]:VAL:HB	1.90	0.54
1:A:445[A]:ILE:HD13	1:A:445[A]:ILE:C	2.28	0.54
1:F:259[A]:GLU:HG2	1:F:264[A]:GLY:HA2	1.90	0.54
1:J:282[A]:PRO:HG2	1:J:301[A]:ARG:HG2	1.90	0.54
2:K:155[A]:ARG:NH1	2:K:157[A]:ILE:HD11	2.22	0.54
1:A:445[C]:ILE:C	1:A:445[C]:ILE:HD13	2.28	0.54
1:F:259[C]:GLU:HG2	1:F:264[C]:GLY:HA2	1.90	0.54
1:J:282[C]:PRO:HG2	1:J:301[C]:ARG:HG2	1.90	0.54
2:K:168[C]:GLN:HG3	2:K:168[C]:GLN:O	2.07	0.54
2:N:167[C]:VAL:O	2:N:168[C]:GLN:C	2.45	0.54
1:F:181[A]:MET:HE2	1:F:197[A]:TRP:CB	2.37	0.53
1:I:259[A]:GLU:HG3	1:I:264[A]:GLY:HA2	1.90	0.53
1:I:330[A]:LYS:O	1:I:334[A]:GLU:HG3	2.06	0.53
1:I:414[A]:ARG:HA	1:I:441[A]:SER:HA	1.90	0.53
1:J:16[A]:PRO:O	4:J:4759[A]:FAD:O1P	2.25	0.53
1:J:44[A]:THR:CG2	4:J:4759[A]:FAD:O2A	2.57	0.53
1:J:122[A]:THR:CG2	1:J:128[A]:THR:HG22	2.38	0.53
1:F:181[C]:MET:HE2	1:F:197[C]:TRP:CB	2.37	0.53
1:I:259[C]:GLU:HG3	1:I:264[C]:GLY:HA2	1.90	0.53
1:I:330[C]:LYS:O	1:I:334[C]:GLU:HG3	2.06	0.53
1:I:414[C]:ARG:HA	1:I:441[C]:SER:HA	1.90	0.53
3:I:4759[C]:FAD:O2A	1:J:44[C]:THR:CG2	2.57	0.53
3:I:4759[C]:FAD:O1P	1:J:16[C]:PRO:O	2.25	0.53
1:J:122[C]:THR:CG2	1:J:128[C]:THR:HG22	2.38	0.53
2:M:141[C]:LYS:O	2:M:141[C]:LYS:HD3	2.06	0.53
2:N:166[C]:LEU:HA	2:N:169[C]:LEU:HD12	1.89	0.53
1:B:160[A]:ILE:CD1	1:B:276[A]:VAL:HB	2.38	0.53
1:B:409[A]:GLN:O	1:B:410[A]:LYS:C	2.44	0.53
1:E:225[A]:ASN:O	1:E:229[A]:ILE:HG12	2.09	0.53
1:E:386[A]:PHE:HZ	1:E:473[A]:ASN:HB2	1.73	0.53
1:G:325[A]:PRO:O	1:G:330[A]:LYS:HE3	2.09	0.53
1:I:229[A]:ILE:HG21	1:I:362[A]:PRO:CG	2.38	0.53
1:I:364[A]:VAL:HG22	1:I:421[A]:LEU:HD12	1.89	0.53
1:B:160[C]:ILE:CD1	1:B:276[C]:VAL:HB	2.38	0.53
1:B:409[C]:GLN:O	1:B:410[C]:LYS:C	2.44	0.53
1:E:225[C]:ASN:O	1:E:229[C]:ILE:HG12	2.09	0.53
1:E:386[C]:PHE:HZ	1:E:473[C]:ASN:HB2	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:325[C]:PRO:O	1:G:330[C]:LYS:HE3	2.09	0.53
1:I:229[C]:ILE:HG21	1:I:362[C]:PRO:CG	2.38	0.53
1:I:364[C]:VAL:HG22	1:I:421[C]:LEU:HD12	1.89	0.53
1:B:461[A]:GLU:OE1	1:B:471[A]:SER:HB2	2.08	0.53
1:C:137[A]:GLN:HE21	1:C:138[A]:VAL:N	2.06	0.53
1:G:357[A]:VAL:HG11	1:G:359[A]:TYR:CE1	2.44	0.53
1:H:19[A]:TYR:C	1:H:19[A]:TYR:CD1	2.81	0.53
1:B:461[C]:GLU:OE1	1:B:471[C]:SER:HB2	2.08	0.53
1:C:137[C]:GLN:HE21	1:C:138[C]:VAL:N	2.06	0.53
1:G:357[C]:VAL:HG11	1:G:359[C]:TYR:CE1	2.44	0.53
1:H:19[C]:TYR:CD1	1:H:19[C]:TYR:C	2.81	0.53
1:A:137[A]:GLN:HE21	1:A:137[A]:GLN:C	2.11	0.53
1:A:238[A]:LYS:HE3	1:A:238[A]:LYS:HA	1.90	0.53
1:C:191[A]:VAL:HG23	1:C:192[A]:GLU:N	2.23	0.53
1:D:198[A]:GLN:NE2	1:D:233[A]:GLN:O	2.40	0.53
1:G:87[A]:LYS:HA	1:G:90[A]:GLU:HB2	1.89	0.53
1:G:336[A]:ILE:O	1:G:340[A]:GLU:HB2	2.09	0.53
2:K:159[A]:THR:O	2:K:162[A]:ASP:HB2	2.08	0.53
1:A:137[C]:GLN:HE21	1:A:137[C]:GLN:C	2.11	0.53
1:A:238[C]:LYS:HE3	1:A:238[C]:LYS:HA	1.90	0.53
1:C:191[C]:VAL:HG23	1:C:192[C]:GLU:N	2.23	0.53
1:D:198[C]:GLN:NE2	1:D:233[C]:GLN:O	2.40	0.53
1:G:87[C]:LYS:HA	1:G:90[C]:GLU:HB2	1.89	0.53
1:G:336[C]:ILE:O	1:G:340[C]:GLU:HB2	2.09	0.53
2:M:159[C]:THR:HG22	2:M:162[C]:ASP:OD1	2.09	0.53
1:E:209[A]:PHE:O	1:E:240[A]:ASN:HA	2.08	0.53
1:F:227[A]:GLN:HE21	1:F:231[A]:GLN:NE2	2.06	0.53
1:G:299[A]:ARG:HD2	1:G:299[A]:ARG:N	2.23	0.53
1:I:24[A]:LYS:HG3	1:I:336[A]:ILE:HG13	1.90	0.53
2:K:159[A]:THR:HG21	2:K:161[A]:GLU:HB2	1.90	0.53
2:M:132[A]:SER:O	2:M:134[A]:ALA:N	2.42	0.53
1:E:209[C]:PHE:O	1:E:240[C]:ASN:HA	2.08	0.53
1:F:227[C]:GLN:HE21	1:F:231[C]:GLN:NE2	2.06	0.53
1:G:299[C]:ARG:HD2	1:G:299[C]:ARG:N	2.23	0.53
1:I:24[C]:LYS:HG3	1:I:336[C]:ILE:HG13	1.90	0.53
1:D:256[A]:VAL:O	1:D:256[A]:VAL:HG23	2.07	0.53
1:E:434[A]:LEU:CD1	1:F:448[A]:VAL:HG21	2.39	0.53
1:D:256[C]:VAL:HG23	1:D:256[C]:VAL:O	2.07	0.53
1:E:434[C]:LEU:CD1	1:F:448[C]:VAL:HG21	2.39	0.53
1:C:158[A]:ILE:H	1:C:158[A]:ILE:CD1	2.20	0.53
1:I:297[A]:ASP:C	1:I:299[A]:ARG:H	2.12	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:396[A]:THR:C	1:I:398[A]:ALA:H	2.10	0.53
1:I:426[A]:GLY:O	1:I:429[A]:VAL:HG12	2.08	0.53
1:J:189[A]:ILE:HG13	4:J:4759[A]:FAD:HM73	1.91	0.53
2:M:159[A]:THR:CG2	2:M:161[A]:GLU:OE1	2.57	0.53
1:C:158[C]:ILE:H	1:C:158[C]:ILE:CD1	2.20	0.53
1:I:297[C]:ASP:C	1:I:299[C]:ARG:H	2.12	0.53
1:I:396[C]:THR:C	1:I:398[C]:ALA:H	2.10	0.53
1:I:426[C]:GLY:O	1:I:429[C]:VAL:HG12	2.08	0.53
3:I:4759[C]:FAD:HM73	1:J:189[C]:ILE:HG13	1.91	0.53
2:L:132[C]:SER:O	2:L:133[C]:PRO:C	2.47	0.53
1:A:229[A]:ILE:O	1:A:233[A]:GLN:HG3	2.08	0.53
1:C:46[A]:LEU:HD11	1:C:99[A]:LEU:HB3	1.90	0.53
1:H:127[A]:VAL:CG2	1:H:144[A]:ILE:CD1	2.82	0.53
1:H:251[A]:ASP:OD2	1:H:253[A]:LYS:HD2	2.08	0.53
1:J:415[A]:VAL:HG23	1:J:415[A]:VAL:O	2.08	0.53
1:A:229[C]:ILE:O	1:A:233[C]:GLN:HG3	2.08	0.53
1:C:46[C]:LEU:HD11	1:C:99[C]:LEU:HB3	1.90	0.53
1:H:127[C]:VAL:CG2	1:H:144[C]:ILE:CD1	2.82	0.53
1:H:251[C]:ASP:OD2	1:H:253[C]:LYS:HD2	2.08	0.53
1:J:415[C]:VAL:HG23	1:J:415[C]:VAL:O	2.08	0.53
1:A:78[A]:MET:HA	1:B:80[A]:GLU:O	2.09	0.53
3:A:4750[A]:FAD:O2'	3:A:4750[A]:FAD:O4'	2.16	0.53
1:B:414[A]:ARG:O	1:B:414[A]:ARG:HG3	2.07	0.53
1:D:213[A]:VAL:HG23	1:D:214[A]:GLY:N	2.24	0.53
1:E:454[A]:THR:HB	1:F:427[A]:GLU:OE2	2.09	0.53
1:H:262[A]:SER:O	1:H:263[A]:GLY:O	2.26	0.53
2:L:138[A]:ILE:HD11	2:L:160[A]:LYS:HE3	1.91	0.53
1:A:78[C]:MET:HA	1:B:80[C]:GLU:O	2.09	0.53
1:B:414[C]:ARG:O	1:B:414[C]:ARG:HG3	2.07	0.53
1:D:213[C]:VAL:HG23	1:D:214[C]:GLY:N	2.24	0.53
1:E:454[C]:THR:HB	1:F:427[C]:GLU:OE2	2.09	0.53
1:H:262[C]:SER:O	1:H:263[C]:GLY:O	2.26	0.53
3:O:4750[C]:FAD:O2'	3:O:4750[C]:FAD:O4'	2.16	0.53
1:C:291[A]:GLU:H	1:C:291[A]:GLU:CD	2.10	0.53
1:C:409[A]:GLN:HB3	1:C:414[A]:ARG:H	1.74	0.53
1:D:224[A]:LYS:HB3	1:D:228[A]:ARG:HH22	1.74	0.53
1:E:409[A]:GLN:HG2	1:E:412[A]:THR:HG23	1.91	0.53
1:F:361[A]:HIS:HA	1:F:362[A]:PRO:C	2.29	0.53
1:H:184[A]:ILE:CD1	1:H:274[A]:LEU:HD11	2.38	0.53
1:I:258[A]:ILE:C	1:I:258[A]:ILE:HD12	2.29	0.53
1:J:184[A]:ILE:HG22	1:J:278[A]:ILE:HG23	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:336[A]:ILE:HG22	1:J:337[A]:ILE:N	2.22	0.53
2:N:142[A]:HIS:C	2:N:144[A]:LEU:H	2.12	0.53
1:C:291[C]:GLU:H	1:C:291[C]:GLU:CD	2.10	0.53
1:C:409[C]:GLN:HB3	1:C:414[C]:ARG:H	1.74	0.53
1:D:224[C]:LYS:HB3	1:D:228[C]:ARG:HH22	1.74	0.53
1:E:409[C]:GLN:HG2	1:E:412[C]:THR:HG23	1.91	0.53
1:F:361[C]:HIS:HA	1:F:362[C]:PRO:C	2.29	0.53
1:H:184[C]:ILE:CD1	1:H:274[C]:LEU:HD11	2.38	0.53
1:I:258[C]:ILE:C	1:I:258[C]:ILE:HD12	2.29	0.53
1:J:184[C]:ILE:HG22	1:J:278[C]:ILE:HG23	1.90	0.53
1:J:336[C]:ILE:HG22	1:J:337[C]:ILE:N	2.22	0.53
1:A:210[A]:LEU:H	1:A:210[A]:LEU:HD22	1.74	0.52
1:A:318[A]:ILE:C	1:A:318[A]:ILE:HD12	2.29	0.52
1:A:447[A]:ARG:HH11	1:A:447[A]:ARG:HG3	1.73	0.52
1:B:23[A]:ILE:O	1:B:27[A]:GLN:HG2	2.08	0.52
1:E:305[A]:ASN:ND2	1:E:307[A]:ARG:N	2.57	0.52
1:G:3[A]:GLN:HB3	1:G:4[A]:PRO:HD2	1.91	0.52
1:H:218[A]:ILE:HG13	1:H:222[A]:ILE:HD11	1.89	0.52
1:A:210[C]:LEU:HD22	1:A:210[C]:LEU:H	1.74	0.52
1:A:318[C]:ILE:C	1:A:318[C]:ILE:HD12	2.29	0.52
1:A:447[C]:ARG:HH11	1:A:447[C]:ARG:HG3	1.73	0.52
1:B:23[C]:ILE:O	1:B:27[C]:GLN:HG2	2.08	0.52
1:E:305[C]:ASN:ND2	1:E:307[C]:ARG:N	2.57	0.52
1:G:3[C]:GLN:HB3	1:G:4[C]:PRO:HD2	1.91	0.52
1:H:218[C]:ILE:HG13	1:H:222[C]:ILE:HD11	1.89	0.52
1:D:305[A]:ASN:ND2	1:D:309[A]:GLN:H	2.07	0.52
1:E:361[A]:HIS:CE1	1:E:399[A]:ASP:OD2	2.63	0.52
1:F:84[A]:ASN:HD22	1:F:84[A]:ASN:C	2.13	0.52
1:H:221[A]:GLU:HB3	1:H:405[A]:LYS:HZ2	1.74	0.52
2:L:144[A]:LEU:HD22	2:L:145[A]:ASP:N	2.23	0.52
1:D:305[C]:ASN:ND2	1:D:309[C]:GLN:H	2.07	0.52
1:E:361[C]:HIS:CE1	1:E:399[C]:ASP:OD2	2.63	0.52
1:F:84[C]:ASN:HD22	1:F:84[C]:ASN:C	2.13	0.52
1:H:221[C]:GLU:HB3	1:H:405[C]:LYS:HZ2	1.74	0.52
1:F:43[A]:GLY:HA2	3:F:4755[A]:FAD:O3B	2.09	0.52
1:G:393[A]:ARG:HH11	1:G:454[A]:THR:HA	1.74	0.52
1:H:446[A]:ALA:O	1:H:460[A]:ARG:NH1	2.42	0.52
1:J:256[A]:VAL:HG11	1:J:274[A]:LEU:HD13	1.89	0.52
2:L:154[A]:PRO:C	2:L:156[A]:GLY:H	2.12	0.52
3:E:4755[C]:FAD:O3B	1:F:43[C]:GLY:HA2	2.09	0.52
1:G:393[C]:ARG:HH11	1:G:454[C]:THR:HA	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:446[C]:ALA:O	1:H:460[C]:ARG:NH1	2.42	0.52
1:J:256[C]:VAL:HG11	1:J:274[C]:LEU:HD13	1.89	0.52
1:A:19[A]:TYR:CD1	1:A:19[A]:TYR:C	2.82	0.52
1:C:297[A]:ASP:HB2	1:C:298[A]:PRO:HD2	1.90	0.52
1:D:171[A]:ALA:HA	1:D:174[A]:LEU:HD13	1.92	0.52
1:D:275[A]:LEU:HD23	1:D:276[A]:VAL:N	2.24	0.52
1:E:20[A]:VAL:CG2	1:E:336[A]:ILE:HD12	2.39	0.52
1:E:46[A]:LEU:HD11	1:E:99[A]:LEU:CB	2.39	0.52
1:I:438[A]:TYR:OH	1:J:440[A]:ALA:HB2	2.10	0.52
1:J:61[A]:HIS:HB2	1:J:199[A]:ARG:NH1	2.25	0.52
1:J:329[A]:HIS:NE2	1:J:355[A]:PRO:O	2.42	0.52
1:A:19[C]:TYR:CD1	1:A:19[C]:TYR:C	2.82	0.52
1:C:297[C]:ASP:HB2	1:C:298[C]:PRO:HD2	1.90	0.52
1:D:171[C]:ALA:HA	1:D:174[C]:LEU:HD13	1.92	0.52
1:D:275[C]:LEU:HD23	1:D:276[C]:VAL:N	2.24	0.52
1:E:20[C]:VAL:CG2	1:E:336[C]:ILE:HD12	2.39	0.52
1:E:46[C]:LEU:HD11	1:E:99[C]:LEU:CB	2.39	0.52
1:I:438[C]:TYR:OH	1:J:440[C]:ALA:HB2	2.10	0.52
1:J:61[C]:HIS:HB2	1:J:199[C]:ARG:NH1	2.25	0.52
1:J:329[C]:HIS:NE2	1:J:355[C]:PRO:O	2.42	0.52
1:E:469[A]:GLY:O	1:E:470[A]:LYS:HB3	2.09	0.52
1:H:221[A]:GLU:HB3	1:H:405[A]:LYS:NZ	2.25	0.52
1:J:195[A]:SER:O	1:J:199[A]:ARG:HG3	2.10	0.52
1:E:469[C]:GLY:O	1:E:470[C]:LYS:HB3	2.09	0.52
1:H:221[C]:GLU:HB3	1:H:405[C]:LYS:NZ	2.25	0.52
1:J:195[C]:SER:O	1:J:199[C]:ARG:HG3	2.10	0.52
1:C:309[A]:GLN:HG2	1:C:316[A]:TYR:CE2	2.45	0.52
1:C:358[A]:ILE:HG23	1:C:364[A]:VAL:HB	1.92	0.52
1:C:449[A]:CYS:HB3	4:D:4809[A]:HOH:O	2.09	0.52
1:G:297[A]:ASP:HB2	1:G:301[A]:ARG:H	1.74	0.52
1:G:448[A]:VAL:HG21	1:H:434[A]:LEU:HD13	1.91	0.52
1:G:454[A]:THR:HB	1:H:427[A]:GLU:OE1	2.08	0.52
1:I:381[A]:TYR:C	1:I:381[A]:TYR:HD1	2.11	0.52
2:M:144[A]:LEU:HD11	2:M:167[A]:VAL:HG22	1.91	0.52
1:C:309[C]:GLN:HG2	1:C:316[C]:TYR:CE2	2.45	0.52
1:C:358[C]:ILE:HG23	1:C:364[C]:VAL:HB	1.92	0.52
1:C:449[C]:CYS:HB3	4:C:4809[C]:HOH:O	2.09	0.52
1:G:297[C]:ASP:HB2	1:G:301[C]:ARG:H	1.74	0.52
1:G:448[C]:VAL:HG21	1:H:434[C]:LEU:HD13	1.91	0.52
1:G:454[C]:THR:HB	1:H:427[C]:GLU:OE1	2.08	0.52
1:I:381[C]:TYR:C	1:I:381[C]:TYR:HD1	2.11	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:144[C]:LEU:N	2:L:144[C]:LEU:HD23	2.24	0.52
1:A:330[A]:LYS:HE2	1:A:334[A]:GLU:OE2	2.10	0.52
1:B:164[A]:THR:HG21	1:B:248[A]:LYS:NZ	2.25	0.52
1:B:218[A]:ILE:HD12	1:B:223[A]:SER:HB2	1.92	0.52
1:B:290[A]:GLU:C	1:B:292[A]:LEU:H	2.12	0.52
1:B:393[A]:ARG:HA	1:B:396[A]:THR:HG22	1.92	0.52
1:D:20[A]:VAL:HG21	1:D:332[A]:GLU:CG	2.37	0.52
1:H:83[A]:LEU:HD13	1:H:84[A]:ASN:N	2.25	0.52
1:H:85[A]:LEU:HD12	1:H:176[A]:LYS:HA	1.92	0.52
1:H:222[A]:ILE:CD1	4:H:4775[A]:HOH:O	2.49	0.52
1:A:330[C]:LYS:HE2	1:A:334[C]:GLU:OE2	2.10	0.52
1:B:164[C]:THR:HG21	1:B:248[C]:LYS:NZ	2.25	0.52
1:B:218[C]:ILE:HD12	1:B:223[C]:SER:HB2	1.92	0.52
1:B:290[C]:GLU:C	1:B:292[C]:LEU:H	2.12	0.52
1:B:393[C]:ARG:HA	1:B:396[C]:THR:HG22	1.92	0.52
1:D:20[C]:VAL:HG21	1:D:332[C]:GLU:CG	2.37	0.52
4:G:4775[C]:HOH:O	1:H:222[C]:ILE:CD1	2.49	0.52
1:H:83[C]:LEU:HD13	1:H:84[C]:ASN:N	2.25	0.52
1:H:85[C]:LEU:HD12	1:H:176[C]:LYS:HA	1.92	0.52
2:K:142[C]:HIS:HB2	2:K:144[C]:LEU:HD12	1.92	0.52
2:N:153[C]:GLY:O	2:N:154[C]:PRO:C	2.47	0.52
1:B:164[A]:THR:CG2	1:B:248[A]:LYS:NZ	2.73	0.52
1:F:124[A]:LYS:HG2	1:F:312[A]:ILE:HD11	1.88	0.52
1:I:43[A]:GLY:O	1:I:47[A]:ASN:HB2	2.10	0.52
1:J:372[A]:GLU:CD	1:J:372[A]:GLU:H	2.11	0.52
1:J:406[A]:ILE:C	1:J:407[A]:LEU:HD23	2.29	0.52
1:B:164[C]:THR:CG2	1:B:248[C]:LYS:NZ	2.73	0.52
1:F:124[C]:LYS:HG2	1:F:312[C]:ILE:HD11	1.88	0.52
1:I:43[C]:GLY:O	1:I:47[C]:ASN:HB2	2.10	0.52
1:J:372[C]:GLU:H	1:J:372[C]:GLU:CD	2.11	0.52
1:J:406[C]:ILE:C	1:J:407[C]:LEU:HD23	2.29	0.52
1:J:96[A]:VAL:O	1:J:100[A]:THR:HG23	2.10	0.52
1:E:348[C]:HIS:HB2	2:M:140[C]:GLU:OE1	2.09	0.52
1:J:96[C]:VAL:O	1:J:100[C]:THR:HG23	2.10	0.52
1:A:137[A]:GLN:CA	1:A:137[A]:GLN:NE2	2.72	0.52
1:A:221[A]:GLU:O	1:A:225[A]:ASN:OD1	2.27	0.52
1:C:442[A]:CYS:HA	1:C:463[A]:ASN:ND2	2.25	0.52
1:J:10[A]:THR:HG23	1:J:33[A]:VAL:CG1	2.40	0.52
2:N:155[A]:ARG:HG2	2:N:156[A]:GLY:N	2.25	0.52
1:A:137[C]:GLN:CA	1:A:137[C]:GLN:NE2	2.72	0.52
1:A:221[C]:GLU:O	1:A:225[C]:ASN:OD1	2.27	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:442[C]:CYS:HA	1:C:463[C]:ASN:ND2	2.25	0.52
1:J:10[C]:THR:HG23	1:J:33[C]:VAL:CG1	2.40	0.52
2:M:154[C]:PRO:C	2:M:156[C]:GLY:N	2.60	0.52
1:C:297[A]:ASP:OD1	1:C:301[A]:ARG:HB2	2.10	0.51
1:E:414[A]:ARG:NH2	1:E:439[A]:GLY:HA2	2.25	0.51
1:G:332[A]:GLU:O	1:G:333[A]:ASP:C	2.46	0.51
1:H:76[A]:ILE:O	1:H:76[A]:ILE:HG22	2.09	0.51
1:J:249[A]:LYS:HE2	1:J:255[A]:ASP:OD1	2.10	0.51
2:K:154[A]:PRO:O	2:K:156[A]:GLY:N	2.43	0.51
1:C:297[C]:ASP:OD1	1:C:301[C]:ARG:HB2	2.10	0.51
1:E:414[C]:ARG:NH2	1:E:439[C]:GLY:HA2	2.25	0.51
1:G:332[C]:GLU:O	1:G:333[C]:ASP:C	2.46	0.51
1:H:76[C]:ILE:O	1:H:76[C]:ILE:HG22	2.09	0.51
1:J:249[C]:LYS:HE2	1:J:255[C]:ASP:OD1	2.10	0.51
1:C:230[A]:LEU:O	1:C:233[A]:GLN:HB2	2.09	0.51
1:E:70[A]:ASP:OD1	1:E:74[A]:ARG:HD2	2.09	0.51
1:F:442[A]:CYS:HB2	1:F:467[A]:SER:HB3	1.92	0.51
1:G:408[A]:GLY:HA2	1:G:414[A]:ARG:O	2.11	0.51
1:I:229[A]:ILE:HG21	1:I:362[A]:PRO:HG3	1.92	0.51
1:I:402[A]:GLY:HA3	1:I:421[A]:LEU:O	2.10	0.51
1:C:230[C]:LEU:O	1:C:233[C]:GLN:HB2	2.09	0.51
1:E:70[C]:ASP:OD1	1:E:74[C]:ARG:HD2	2.09	0.51
1:F:442[C]:CYS:HB2	1:F:467[C]:SER:HB3	1.92	0.51
1:G:408[C]:GLY:HA2	1:G:414[C]:ARG:O	2.11	0.51
1:I:229[C]:ILE:HG21	1:I:362[C]:PRO:HG3	1.92	0.51
1:I:402[C]:GLY:HA3	1:I:421[C]:LEU:O	2.10	0.51
2:L:132[C]:SER:OG	2:L:135[C]:ALA:N	2.32	0.51
1:A:125[A]:ASN:HB3	1:A:141[A]:THR:O	2.10	0.51
1:D:10[A]:THR:HG21	1:D:139[A]:ILE:HG21	1.92	0.51
1:G:358[A]:ILE:CD1	1:G:360[A]:THR:OG1	2.57	0.51
1:I:358[A]:ILE:O	1:I:358[A]:ILE:HG12	2.09	0.51
1:A:125[C]:ASN:HB3	1:A:141[C]:THR:O	2.10	0.51
1:A:444[C]:ASP:OD2	2:K:155[C]:ARG:NH2	2.43	0.51
1:B:438[C]:TYR:CE1	2:K:157[C]:ILE:HD11	2.46	0.51
1:D:10[C]:THR:HG21	1:D:139[C]:ILE:HG21	1.92	0.51
1:G:358[C]:ILE:CD1	1:G:360[C]:THR:OG1	2.57	0.51
1:I:358[C]:ILE:O	1:I:358[C]:ILE:HG12	2.09	0.51
1:B:6[A]:ASP:HA	1:B:140[A]:ASP:O	2.10	0.51
1:B:256[A]:VAL:CG2	1:B:269[A]:ILE:HB	2.40	0.51
1:D:461[A]:GLU:OE1	1:D:464[A]:LEU:HD23	2.10	0.51
1:G:35[A]:ILE:HD12	1:G:35[A]:ILE:N	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:307[A]:ARG:O	1:H:308[A]:PHE:HB2	2.10	0.51
1:H:385[A]:LYS:HE2	1:H:403[A]:MET:HE1	1.92	0.51
1:I:208[A]:GLU:OE1	1:I:208[A]:GLU:HA	2.10	0.51
1:B:6[C]:ASP:HA	1:B:140[C]:ASP:O	2.10	0.51
1:B:256[C]:VAL:CG2	1:B:269[C]:ILE:HB	2.40	0.51
1:D:461[C]:GLU:OE1	1:D:464[C]:LEU:HD23	2.10	0.51
1:G:35[C]:ILE:HD12	1:G:35[C]:ILE:N	2.26	0.51
1:H:307[C]:ARG:O	1:H:308[C]:PHE:HB2	2.10	0.51
1:H:385[C]:LYS:HE2	1:H:403[C]:MET:HE1	1.92	0.51
1:I:208[C]:GLU:OE1	1:I:208[C]:GLU:HA	2.10	0.51
1:A:145[A]:LEU:HD21	1:A:318[A]:ILE:CG1	2.41	0.51
1:C:166[A]:VAL:HB	1:C:170[A]:GLY:HA3	1.91	0.51
1:D:316[A]:TYR:N	1:D:316[A]:TYR:CD1	2.79	0.51
1:A:145[C]:LEU:HD21	1:A:318[C]:ILE:CG1	2.41	0.51
1:C:166[C]:VAL:HB	1:C:170[C]:GLY:HA3	1.91	0.51
1:D:316[C]:TYR:N	1:D:316[C]:TYR:CD1	2.79	0.51
2:K:162[C]:ASP:O	2:K:166[C]:LEU:HD23	2.11	0.51
2:M:132[C]:SER:O	2:M:133[C]:PRO:C	2.49	0.51
1:A:46[A]:LEU:HG	1:A:100[A]:THR:HG22	1.93	0.51
1:A:189[A]:ILE:HG23	3:A:4750[A]:FAD:HM73	1.92	0.51
1:B:256[A]:VAL:O	1:B:256[A]:VAL:CG2	2.58	0.51
1:D:102[A]:GLY:O	1:D:105[A]:HIS:HB3	2.11	0.51
1:D:368[A]:GLY:HA3	1:D:417[A]:GLY:HA2	1.93	0.51
1:E:420[A]:ILE:HB	1:E:425[A]:ALA:HB1	1.93	0.51
1:I:78[A]:MET:SD	1:J:78[A]:MET:CE	2.99	0.51
1:I:78[A]:MET:CE	1:J:78[A]:MET:HE3	2.41	0.51
1:A:46[C]:LEU:HG	1:A:100[C]:THR:HG22	1.93	0.51
1:A:189[C]:ILE:HG23	3:O:4750[C]:FAD:HM73	1.92	0.51
1:B:256[C]:VAL:O	1:B:256[C]:VAL:CG2	2.58	0.51
1:D:102[C]:GLY:O	1:D:105[C]:HIS:HB3	2.11	0.51
1:D:368[C]:GLY:HA3	1:D:417[C]:GLY:HA2	1.93	0.51
1:E:420[C]:ILE:HB	1:E:425[C]:ALA:HB1	1.93	0.51
1:I:78[C]:MET:SD	1:J:78[C]:MET:CE	2.99	0.51
1:I:78[C]:MET:CE	1:J:78[C]:MET:HE3	2.41	0.51
1:D:183[A]:VAL:CG1	1:D:275[A]:LEU:HD13	2.40	0.51
1:E:431[A]:GLU:OE2	1:E:450[A]:HIS:NE2	2.26	0.51
1:G:51[A]:ILE:HB	1:G:52[A]:PRO:HD3	1.91	0.51
1:G:57[A]:LEU:HD13	1:G:359[A]:TYR:O	2.10	0.51
1:G:254[A]:ILE:HD12	1:G:255[A]:ASP:H	1.76	0.51
1:G:259[A]:GLU:OE2	1:G:264[A]:GLY:CA	2.59	0.51
1:H:45[A]:CYS:SG	1:H:50[A]:CYS:HB2	2.50	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:195[A]:SER:O	1:I:199[A]:ARG:HG3	2.10	0.51
1:I:428[A]:MET:HE1	1:I:455[A]:LEU:C	2.31	0.51
2:O:158[A]:PHE:CZ	2:O:166[A]:LEU:HD12	2.39	0.51
1:D:183[C]:VAL:CG1	1:D:275[C]:LEU:HD13	2.40	0.51
1:E:431[C]:GLU:OE2	1:E:450[C]:HIS:NE2	2.26	0.51
1:G:51[C]:ILE:HB	1:G:52[C]:PRO:HD3	1.91	0.51
1:G:57[C]:LEU:HD13	1:G:359[C]:TYR:O	2.10	0.51
1:G:254[C]:ILE:HD12	1:G:255[C]:ASP:H	1.76	0.51
1:G:259[C]:GLU:OE2	1:G:264[C]:GLY:CA	2.59	0.51
1:H:45[C]:CYS:SG	1:H:50[C]:CYS:HB2	2.50	0.51
1:I:195[C]:SER:O	1:I:199[C]:ARG:HG3	2.10	0.51
1:I:428[C]:MET:HE1	1:I:455[C]:LEU:C	2.31	0.51
1:B:124[A]:LYS:HG3	1:B:125[A]:ASN:ND2	2.26	0.51
1:C:392[A]:SER:HB2	4:C:4813[A]:HOH:O	2.11	0.51
1:E:276[A]:VAL:HG12	4:E:4762[A]:HOH:O	2.10	0.51
1:E:366[A]:TRP:CB	1:E:419[A]:HIS:CD2	2.91	0.51
1:F:143[A]:ASN:ND2	1:F:342[A]:MET:CE	2.73	0.51
1:H:52[A]:PRO:O	1:H:55[A]:ALA:HB3	2.11	0.51
1:H:349[A]:ILE:HG22	4:H:4803[A]:HOH:O	2.10	0.51
1:J:54[A]:LYS:HD2	1:J:359[A]:TYR:CD1	2.46	0.51
1:B:124[C]:LYS:HG3	1:B:125[C]:ASN:ND2	2.26	0.51
4:B:4813[C]:HOH:O	1:C:392[C]:SER:HB2	2.11	0.51
4:D:4762[C]:HOH:O	1:E:276[C]:VAL:HG12	2.10	0.51
1:E:366[C]:TRP:CB	1:E:419[C]:HIS:CD2	2.91	0.51
1:F:143[C]:ASN:ND2	1:F:342[C]:MET:CE	2.73	0.51
4:G:4803[C]:HOH:O	1:H:349[C]:ILE:HG22	2.10	0.51
1:H:52[C]:PRO:O	1:H:55[C]:ALA:HB3	2.11	0.51
1:J:54[C]:LYS:HD2	1:J:359[C]:TYR:CD1	2.46	0.51
2:L:132[C]:SER:OG	2:L:135[C]:ALA:HB2	2.11	0.51
2:L:132[C]:SER:CB	2:L:135[C]:ALA:HB2	2.41	0.51
2:M:154[C]:PRO:C	2:M:156[C]:GLY:H	2.14	0.51
1:A:253[A]:LYS:HE2	1:A:270[A]:THR:OG1	2.11	0.51
1:E:88[A]:MET:HE2	1:E:200[A]:LEU:HD21	1.92	0.51
1:G:267[A]:GLU:HG2	1:G:268[A]:VAL:N	2.24	0.51
1:I:46[A]:LEU:CD2	1:I:100[A]:THR:HG22	2.41	0.51
1:I:88[A]:MET:HE2	1:I:200[A]:LEU:HD11	1.93	0.51
1:J:222[A]:ILE:HG13	1:J:223[A]:SER:N	2.25	0.51
1:A:253[C]:LYS:HE2	1:A:270[C]:THR:OG1	2.11	0.51
1:D:443[C]:GLU:HG2	2:L:134[C]:ALA:CB	2.40	0.51
1:E:88[C]:MET:HE2	1:E:200[C]:LEU:HD21	1.92	0.51
1:G:267[C]:GLU:HG2	1:G:268[C]:VAL:N	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:46[C]:LEU:CD2	1:I:100[C]:THR:HG22	2.41	0.51
1:I:88[C]:MET:HE2	1:I:200[C]:LEU:HD11	1.93	0.51
1:J:222[C]:ILE:HG13	1:J:223[C]:SER:N	2.25	0.51
2:N:137[C]:ASN:O	2:N:138[C]:ILE:C	2.49	0.51
1:C:44[A]:THR:O	1:C:49[A]:GLY:N	2.44	0.51
1:C:225[A]:ASN:HA	1:C:228[A]:ARG:HH11	1.76	0.51
1:C:326[A]:MET:CE	1:C:326[A]:MET:CG	2.88	0.51
1:C:430[A]:ASN:HD22	1:D:456[A]:SER:HB3	1.74	0.51
1:E:46[A]:LEU:CD2	1:E:100[A]:THR:HG22	2.40	0.51
1:H:307[A]:ARG:HB3	1:H:347[A]:VAL:HG21	1.92	0.51
1:I:361[A]:HIS:HA	1:I:362[A]:PRO:C	2.30	0.51
1:I:376[A]:GLU:C	1:I:378[A]:GLY:N	2.65	0.51
1:J:151[A]:GLU:OE2	1:J:281[A]:ARG:NH1	2.38	0.51
1:C:44[C]:THR:O	1:C:49[C]:GLY:N	2.44	0.51
1:C:225[C]:ASN:HA	1:C:228[C]:ARG:HH11	1.76	0.51
1:C:326[C]:MET:CE	1:C:326[C]:MET:CG	2.88	0.51
1:C:430[C]:ASN:HD22	1:D:456[C]:SER:HB3	1.74	0.51
1:E:46[C]:LEU:CD2	1:E:100[C]:THR:HG22	2.40	0.51
1:H:307[C]:ARG:HB3	1:H:347[C]:VAL:HG21	1.92	0.51
1:I:361[C]:HIS:HA	1:I:362[C]:PRO:C	2.30	0.51
1:I:376[C]:GLU:C	1:I:378[C]:GLY:N	2.65	0.51
1:J:151[C]:GLU:OE2	1:J:281[C]:ARG:NH1	2.38	0.51
1:A:167[A]:SER:O	1:A:168[A]:SER:C	2.50	0.50
1:B:122[A]:THR:HG21	1:B:128[A]:THR:OG1	2.11	0.50
1:C:409[A]:GLN:CG	1:C:412[A]:THR:OG1	2.59	0.50
1:E:366[A]:TRP:HB2	1:E:419[A]:HIS:HD2	1.75	0.50
1:F:1[A]:ALA:H1	1:F:136[A]:THR:HG22	1.74	0.50
1:H:409[A]:GLN:HB2	1:H:416[A]:LEU:HD11	1.93	0.50
1:I:396[A]:THR:C	1:I:398[A]:ALA:N	2.64	0.50
1:I:409[A]:GLN:CG	1:I:412[A]:THR:OG1	2.45	0.50
2:L:145[A]:ASP:HB3	2:L:148[A]:GLN:OE1	2.11	0.50
1:A:167[C]:SER:O	1:A:168[C]:SER:C	2.50	0.50
1:B:122[C]:THR:HG21	1:B:128[C]:THR:OG1	2.11	0.50
1:C:409[C]:GLN:CG	1:C:412[C]:THR:OG1	2.59	0.50
1:E:366[C]:TRP:HB2	1:E:419[C]:HIS:HD2	1.75	0.50
1:F:1[C]:ALA:H1	1:F:136[C]:THR:HG22	1.74	0.50
1:H:409[C]:GLN:HB2	1:H:416[C]:LEU:HD11	1.93	0.50
1:I:396[C]:THR:C	1:I:398[C]:ALA:N	2.64	0.50
1:I:409[C]:GLN:CG	1:I:412[C]:THR:OG1	2.45	0.50
1:A:182[A]:VAL:HG21	1:A:256[A]:VAL:HG11	1.92	0.50
1:A:438[A]:TYR:CE1	2:K:157[A]:ILE:HD11	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:87[A]:LYS:HB3	1:D:75[A]:GLY:HA2	1.93	0.50
1:E:304[A]:VAL:CG1	1:E:317[A]:ALA:HB3	2.42	0.50
1:I:388[A]:PHE:CD2	1:I:422[A]:GLY:HA3	2.45	0.50
1:J:335[A]:GLY:O	1:J:339[A]:VAL:HG23	2.12	0.50
1:A:182[C]:VAL:HG21	1:A:256[C]:VAL:HG11	1.92	0.50
1:C:87[C]:LYS:HB3	1:D:75[C]:GLY:HA2	1.93	0.50
1:E:304[C]:VAL:CG1	1:E:317[C]:ALA:HB3	2.42	0.50
1:I:388[C]:PHE:CD2	1:I:422[C]:GLY:HA3	2.45	0.50
1:J:335[C]:GLY:O	1:J:339[C]:VAL:HG23	2.12	0.50
1:A:203[A]:ASP:C	1:A:203[A]:ASP:OD1	2.50	0.50
1:A:218[A]:ILE:HG13	1:A:366[A]:TRP:CZ3	2.46	0.50
1:D:188[A]:VAL:HG12	1:D:189[A]:ILE:N	2.26	0.50
1:E:455[A]:LEU:N	1:F:427[A]:GLU:OE2	2.42	0.50
1:J:46[A]:LEU:HA	1:J:51[A]:ILE:HG12	1.94	0.50
1:A:203[C]:ASP:C	1:A:203[C]:ASP:OD1	2.50	0.50
1:A:218[C]:ILE:HG13	1:A:366[C]:TRP:CZ3	2.46	0.50
1:D:188[C]:VAL:HG12	1:D:189[C]:ILE:N	2.26	0.50
1:E:455[C]:LEU:N	1:F:427[C]:GLU:OE2	2.42	0.50
1:J:46[C]:LEU:HA	1:J:51[C]:ILE:HG12	1.94	0.50
2:M:152[C]:THR:N	2:M:162[C]:ASP:OD2	2.43	0.50
1:E:412[A]:THR:O	1:E:413[A]:ASP:CB	2.58	0.50
1:H:339[A]:VAL:HG23	1:H:340[A]:GLU:N	2.25	0.50
1:I:284[A]:THR:CG2	1:I:289[A]:LEU:HD21	2.41	0.50
1:J:17[A]:GLY:H	1:J:20[A]:VAL:HG23	1.74	0.50
2:L:139[A]:LEU:C	2:L:141[A]:LYS:N	2.65	0.50
2:N:167[A]:VAL:HG12	2:N:168[A]:GLN:N	2.27	0.50
1:E:412[C]:THR:O	1:E:413[C]:ASP:CB	2.58	0.50
1:H:339[C]:VAL:HG23	1:H:340[C]:GLU:N	2.25	0.50
1:I:284[C]:THR:CG2	1:I:289[C]:LEU:HD21	2.41	0.50
1:J:17[C]:GLY:H	1:J:20[C]:VAL:HG23	1.74	0.50
1:A:219[A]:ASP:HB3	1:A:222[A]:ILE:CD1	2.42	0.50
1:B:445[A]:ILE:H	1:B:445[A]:ILE:HD12	1.76	0.50
1:C:158[A]:ILE:HG13	1:C:246[A]:ALA:HB3	1.94	0.50
1:D:432[A]:ALA:O	1:D:436[A]:LEU:HD23	2.11	0.50
1:E:143[A]:ASN:HD22	1:E:342[A]:MET:HE2	1.77	0.50
1:F:121[A]:ILE:HD11	1:F:146[A]:ILE:CD1	2.41	0.50
1:G:358[A]:ILE:HD11	1:G:360[A]:THR:OG1	2.11	0.50
1:H:178[A]:PRO:HB3	1:H:273[A]:VAL:CG2	2.42	0.50
1:I:65[A]:MET:HE2	1:I:71[A]:PHE:HE1	1.77	0.50
1:J:308[A]:PHE:CE1	1:J:334[A]:GLU:HG2	2.47	0.50
2:N:142[A]:HIS:O	2:N:144[A]:LEU:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219[C]:ASP:HB3	1:A:222[C]:ILE:CD1	2.42	0.50
1:B:438[C]:TYR:C	2:K:154[C]:PRO:HG2	2.32	0.50
1:B:445[C]:ILE:H	1:B:445[C]:ILE:HD12	1.76	0.50
1:C:158[C]:ILE:HG13	1:C:246[C]:ALA:HB3	1.94	0.50
1:D:432[C]:ALA:O	1:D:436[C]:LEU:HD23	2.11	0.50
1:E:143[C]:ASN:HD22	1:E:342[C]:MET:HE2	1.77	0.50
1:F:121[C]:ILE:HD11	1:F:146[C]:ILE:CD1	2.41	0.50
1:G:358[C]:ILE:HD11	1:G:360[C]:THR:OG1	2.11	0.50
1:H:178[C]:PRO:HB3	1:H:273[C]:VAL:CG2	2.42	0.50
1:I:65[C]:MET:HE2	1:I:71[C]:PHE:HE1	1.77	0.50
1:J:308[C]:PHE:CE1	1:J:334[C]:GLU:HG2	2.47	0.50
1:E:15[A]:GLY:O	1:E:17[A]:GLY:O	2.29	0.50
1:J:382[A]:LYS:HG2	1:J:408[A]:GLY:O	2.11	0.50
2:M:161[A]:GLU:N	2:M:161[A]:GLU:OE1	2.44	0.50
2:O:131[A]:LEU:HD23	2:O:135[A]:ALA:HB3	1.92	0.50
1:E:15[C]:GLY:O	1:E:17[C]:GLY:O	2.29	0.50
1:J:382[C]:LYS:HG2	1:J:408[C]:GLY:O	2.11	0.50
2:L:159[C]:THR:O	2:L:160[C]:LYS:C	2.50	0.50
1:A:137[A]:GLN:NE2	1:A:137[A]:GLN:HA	2.27	0.50
1:B:288[A]:GLY:HA2	1:B:291[A]:GLU:OE1	2.11	0.50
1:B:393[A]:ARG:HD2	1:B:454[A]:THR:HA	1.94	0.50
1:E:325[A]:PRO:O	1:E:330[A]:LYS:HD2	2.12	0.50
1:G:213[A]:VAL:HG12	1:G:214[A]:GLY:H	1.77	0.50
1:G:305[A]:ASN:ND2	1:G:309[A]:GLN:HG3	2.26	0.50
1:H:364[A]:VAL:HG22	1:H:421[A]:LEU:HD13	1.93	0.50
1:J:97[A]:LYS:O	1:J:98[A]:ALA:C	2.49	0.50
2:L:132[A]:SER:HB2	2:L:135[A]:ALA:CB	2.42	0.50
1:A:137[C]:GLN:NE2	1:A:137[C]:GLN:HA	2.27	0.50
1:B:288[C]:GLY:HA2	1:B:291[C]:GLU:OE1	2.11	0.50
1:B:393[C]:ARG:HD2	1:B:454[C]:THR:HA	1.94	0.50
1:E:325[C]:PRO:O	1:E:330[C]:LYS:HD2	2.12	0.50
1:G:213[C]:VAL:HG12	1:G:214[C]:GLY:H	1.77	0.50
1:G:305[C]:ASN:ND2	1:G:309[C]:GLN:HG3	2.26	0.50
1:H:364[C]:VAL:HG22	1:H:421[C]:LEU:HD13	1.93	0.50
1:J:97[C]:LYS:O	1:J:98[C]:ALA:C	2.49	0.50
1:B:174[A]:LEU:HB2	1:B:197[A]:TRP:CZ2	2.47	0.50
1:D:249[A]:LYS:HD3	1:D:255[A]:ASP:HB2	1.94	0.50
1:E:85[A]:LEU:HD13	1:E:176[A]:LYS:HA	1.93	0.50
1:F:17[A]:GLY:O	1:F:21[A]:ALA:CB	2.59	0.50
1:G:474[A]:PHE:CD2	1:G:474[A]:PHE:O	2.64	0.50
1:I:296[A]:LEU:O	1:I:297[A]:ASP:O	2.30	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:319[A]:GLY:HA3	4:J:4760[A]:HOH:O	2.11	0.50
1:B:174[C]:LEU:HB2	1:B:197[C]:TRP:CZ2	2.47	0.50
1:D:249[C]:LYS:HD3	1:D:255[C]:ASP:HB2	1.94	0.50
1:E:85[C]:LEU:HD13	1:E:176[C]:LYS:HA	1.93	0.50
1:F:17[C]:GLY:O	1:F:21[C]:ALA:CB	2.59	0.50
1:G:474[C]:PHE:O	1:G:474[C]:PHE:CD2	2.64	0.50
1:I:296[C]:LEU:O	1:I:297[C]:ASP:O	2.30	0.50
4:I:4760[C]:HOH:O	1:J:319[C]:GLY:HA3	2.11	0.50
1:A:177[A]:VAL:HG22	1:A:197[A]:TRP:CZ3	2.47	0.50
1:D:145[A]:LEU:HD12	1:D:316[A]:TYR:HB2	1.94	0.50
1:H:409[A]:GLN:N	1:H:416[A]:LEU:CD1	2.75	0.50
1:A:177[C]:VAL:HG22	1:A:197[C]:TRP:CZ3	2.47	0.50
1:D:145[C]:LEU:HD12	1:D:316[C]:TYR:HB2	1.94	0.50
1:H:409[C]:GLN:N	1:H:416[C]:LEU:CD1	2.75	0.50
2:M:153[C]:GLY:O	2:M:154[C]:PRO:C	2.51	0.50
1:A:155[A]:PHE:CZ	1:A:243[A]:VAL:HG22	2.47	0.49
1:B:326[A]:MET:CE	1:B:326[A]:MET:CG	2.89	0.49
1:C:347[A]:VAL:O	1:C:347[A]:VAL:CG2	2.60	0.49
1:D:83[A]:LEU:HD11	1:D:200[A]:LEU:HG	1.93	0.49
1:E:84[A]:ASN:HB2	1:F:77[A]:GLU:HG2	1.93	0.49
1:E:336[A]:ILE:O	1:E:340[A]:GLU:HB2	2.11	0.49
1:F:335[A]:GLY:O	1:F:339[A]:VAL:HG13	2.12	0.49
1:G:322[A]:VAL:HG13	1:G:323[A]:ALA:N	2.27	0.49
1:G:472[A]:ILE:C	1:G:472[A]:ILE:CD1	2.70	0.49
1:H:121[A]:ILE:CG1	1:H:144[A]:ILE:HD11	2.41	0.49
1:I:330[A]:LYS:HE2	1:I:334[A]:GLU:OE2	2.11	0.49
2:M:168[A]:GLN:O	2:M:171[A]:GLN:CG	2.60	0.49
1:A:155[C]:PHE:CZ	1:A:243[C]:VAL:HG22	2.47	0.49
1:B:326[C]:MET:CE	1:B:326[C]:MET:CG	2.89	0.49
1:C:347[C]:VAL:O	1:C:347[C]:VAL:CG2	2.60	0.49
1:D:83[C]:LEU:HD11	1:D:200[C]:LEU:HG	1.93	0.49
1:E:84[C]:ASN:HB2	1:F:77[C]:GLU:HG2	1.93	0.49
1:E:336[C]:ILE:O	1:E:340[C]:GLU:HB2	2.11	0.49
1:F:335[C]:GLY:O	1:F:339[C]:VAL:HG13	2.12	0.49
1:G:322[C]:VAL:HG13	1:G:323[C]:ALA:N	2.27	0.49
1:G:472[C]:ILE:C	1:G:472[C]:ILE:CD1	2.70	0.49
1:H:121[C]:ILE:CG1	1:H:144[C]:ILE:HD11	2.41	0.49
1:I:330[C]:LYS:HE2	1:I:334[C]:GLU:OE2	2.11	0.49
1:C:88[A]:MET:HE3	1:C:200[A]:LEU:HD21	1.93	0.49
1:C:285[A]:LYS:HB3	1:C:285[A]:LYS:NZ	2.27	0.49
1:D:1[A]:ALA:CB	1:D:136[A]:THR:HG23	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:94[A]:THR:HG22	1:E:95[A]:ALA:N	2.27	0.49
1:G:265[A]:LYS:O	1:G:266[A]:ALA:C	2.51	0.49
1:G:343[A]:ALA:O	1:G:344[A]:GLY:C	2.49	0.49
1:I:150[A]:SER:HB2	1:I:281[A]:ARG:O	2.12	0.49
1:I:295[A]:GLU:OE1	1:I:295[A]:GLU:HA	2.11	0.49
2:O:167[A]:VAL:O	2:O:170[A]:LYS:HB3	2.12	0.49
1:C:88[C]:MET:HE3	1:C:200[C]:LEU:HD21	1.93	0.49
1:C:285[C]:LYS:NZ	1:C:285[C]:LYS:HB3	2.27	0.49
1:D:1[C]:ALA:CB	1:D:136[C]:THR:HG23	2.42	0.49
1:E:94[C]:THR:HG22	1:E:95[C]:ALA:N	2.27	0.49
1:G:265[C]:LYS:O	1:G:266[C]:ALA:C	2.51	0.49
1:G:343[C]:ALA:O	1:G:344[C]:GLY:C	2.49	0.49
1:I:150[C]:SER:HB2	1:I:281[C]:ARG:O	2.12	0.49
1:I:295[C]:GLU:OE1	1:I:295[C]:GLU:HA	2.11	0.49
1:A:219[A]:ASP:HB3	1:A:222[A]:ILE:HD13	1.94	0.49
1:B:19[A]:TYR:CD1	1:B:19[A]:TYR:C	2.84	0.49
1:B:453[A]:PRO:HA	1:B:457[A]:GLU:OE2	2.12	0.49
1:D:382[A]:LYS:HE2	1:D:466[A]:ALA:O	2.12	0.49
1:F:59[A]:ASN:OD1	1:F:91[A]:GLN:HG2	2.11	0.49
1:J:92[A]:LYS:HG2	1:J:93[A]:SER:N	2.27	0.49
1:J:179[A]:GLU:HB3	1:J:272[A]:ASP:OD1	2.12	0.49
2:L:158[A]:PHE:HZ	2:L:166[A]:LEU:HD12	1.75	0.49
2:M:135[A]:ALA:HA	2:M:138[A]:ILE:CG1	2.42	0.49
2:M:151[A]:ALA:HB2	2:M:158[A]:PHE:CD1	2.46	0.49
1:A:219[C]:ASP:HB3	1:A:222[C]:ILE:HD13	1.94	0.49
1:B:19[C]:TYR:CD1	1:B:19[C]:TYR:C	2.84	0.49
1:B:453[C]:PRO:HA	1:B:457[C]:GLU:OE2	2.12	0.49
1:D:382[C]:LYS:HE2	1:D:466[C]:ALA:O	2.12	0.49
1:F:59[C]:ASN:OD1	1:F:91[C]:GLN:HG2	2.11	0.49
1:F:444[C]:ASP:OD1	2:M:134[C]:ALA:HB3	2.11	0.49
1:J:92[C]:LYS:HG2	1:J:93[C]:SER:N	2.27	0.49
1:J:179[C]:GLU:HB3	1:J:272[C]:ASP:OD1	2.12	0.49
2:L:132[C]:SER:OG	2:L:135[C]:ALA:CB	2.60	0.49
2:L:144[C]:LEU:HD23	2:L:144[C]:LEU:H	1.77	0.49
1:C:203[A]:ASP:HA	4:C:4809[A]:HOH:O	2.11	0.49
1:D:110[A]:ASN:O	1:D:111[A]:LYS:HB2	2.11	0.49
1:D:278[A]:ILE:O	1:D:278[A]:ILE:HG22	2.12	0.49
3:E:4754[A]:FAD:O2'	3:E:4754[A]:FAD:O4'	2.16	0.49
1:G:33[A]:VAL:HG21	1:G:139[A]:ILE:HG12	1.94	0.49
1:G:213[A]:VAL:HG12	1:G:214[A]:GLY:N	2.28	0.49
1:H:265[A]:LYS:HZ2	1:H:265[A]:LYS:CB	2.16	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:132[A]:SER:O	2:K:133[A]:PRO:C	2.51	0.49
4:B:4809[C]:HOH:O	1:C:203[C]:ASP:HA	2.11	0.49
1:D:110[C]:ASN:O	1:D:111[C]:LYS:HB2	2.11	0.49
1:D:278[C]:ILE:O	1:D:278[C]:ILE:HG22	2.12	0.49
3:D:4754[C]:FAD:O2'	3:D:4754[C]:FAD:O4'	2.16	0.49
1:G:33[C]:VAL:HG21	1:G:139[C]:ILE:HG12	1.94	0.49
1:G:213[C]:VAL:HG12	1:G:214[C]:GLY:N	2.28	0.49
1:H:265[C]:LYS:HZ2	1:H:265[C]:LYS:CB	2.16	0.49
1:B:181[A]:MET:O	1:B:204[A]:VAL:HA	2.12	0.49
1:B:207[A]:VAL:HG13	1:B:241[A]:THR:HB	1.94	0.49
1:B:291[A]:GLU:CD	1:B:291[A]:GLU:N	2.62	0.49
1:C:131[A]:LYS:NZ	1:C:132[A]:ALA:HB3	2.27	0.49
1:C:394[A]:ALA:HB1	1:C:400[A]:THR:HG22	1.94	0.49
1:C:414[A]:ARG:HG2	1:C:414[A]:ARG:NH1	2.22	0.49
1:G:195[A]:SER:O	1:G:199[A]:ARG:HG3	2.13	0.49
1:J:69[A]:LYS:HB2	1:J:69[A]:LYS:NZ	2.27	0.49
1:B:181[C]:MET:O	1:B:204[C]:VAL:HA	2.12	0.49
1:B:207[C]:VAL:HG13	1:B:241[C]:THR:HB	1.94	0.49
1:B:291[C]:GLU:CD	1:B:291[C]:GLU:N	2.62	0.49
1:C:131[C]:LYS:NZ	1:C:132[C]:ALA:HB3	2.27	0.49
1:C:394[C]:ALA:HB1	1:C:400[C]:THR:HG22	1.94	0.49
1:C:414[C]:ARG:HG2	1:C:414[C]:ARG:NH1	2.22	0.49
1:G:195[C]:SER:O	1:G:199[C]:ARG:HG3	2.13	0.49
1:J:69[C]:LYS:HB2	1:J:69[C]:LYS:NZ	2.27	0.49
1:A:358[A]:ILE:CD1	1:A:360[A]:THR:CG2	2.85	0.49
1:E:165[A]:ILE:HG22	1:E:165[A]:ILE:O	2.13	0.49
1:F:84[A]:ASN:C	1:F:84[A]:ASN:ND2	2.64	0.49
1:F:123[A]:GLY:O	1:F:124[A]:LYS:C	2.51	0.49
1:G:136[A]:THR:HG23	1:G:136[A]:THR:O	2.13	0.49
1:G:339[A]:VAL:C	1:G:341[A]:GLY:N	2.64	0.49
1:H:385[A]:LYS:HG2	1:H:403[A]:MET:HE2	1.93	0.49
1:J:428[A]:MET:CE	1:J:455[A]:LEU:HB3	2.42	0.49
1:A:358[C]:ILE:CD1	1:A:360[C]:THR:CG2	2.85	0.49
1:E:165[C]:ILE:HG22	1:E:165[C]:ILE:O	2.13	0.49
1:F:84[C]:ASN:C	1:F:84[C]:ASN:ND2	2.64	0.49
1:F:123[C]:GLY:O	1:F:124[C]:LYS:C	2.51	0.49
1:G:136[C]:THR:HG23	1:G:136[C]:THR:O	2.13	0.49
1:G:339[C]:VAL:C	1:G:341[C]:GLY:N	2.64	0.49
1:H:385[C]:LYS:HG2	1:H:403[C]:MET:HE2	1.93	0.49
1:J:428[C]:MET:CE	1:J:455[C]:LEU:HB3	2.42	0.49
1:A:443[A]:GLU:HB2	2:K:160[A]:LYS:HZ3	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:267[A]:GLU:HG2	1:B:268[A]:VAL:N	2.26	0.49
1:D:218[A]:ILE:HD13	1:D:223[A]:SER:HB2	1.95	0.49
1:D:221[A]:GLU:O	1:D:225[A]:ASN:ND2	2.46	0.49
1:G:291[A]:GLU:OE1	1:G:291[A]:GLU:N	2.43	0.49
1:G:430[A]:ASN:ND2	1:H:451[A]:ALA:H	2.11	0.49
1:H:121[A]:ILE:HG21	1:H:292[A]:LEU:HD21	1.94	0.49
1:I:40[A]:THR:CG2	1:I:100[A]:THR:HB	2.41	0.49
1:I:258[A]:ILE:HD11	1:I:267[A]:GLU:HB3	1.94	0.49
1:B:267[C]:GLU:HG2	1:B:268[C]:VAL:N	2.26	0.49
1:D:218[C]:ILE:HD13	1:D:223[C]:SER:HB2	1.95	0.49
1:D:221[C]:GLU:O	1:D:225[C]:ASN:ND2	2.46	0.49
1:G:291[C]:GLU:N	1:G:291[C]:GLU:OE1	2.43	0.49
1:G:430[C]:ASN:ND2	1:H:451[C]:ALA:H	2.11	0.49
1:H:121[C]:ILE:HG21	1:H:292[C]:LEU:HD21	1.94	0.49
1:I:40[C]:THR:CG2	1:I:100[C]:THR:HB	2.41	0.49
1:I:258[C]:ILE:HD11	1:I:267[C]:GLU:HB3	1.94	0.49
2:N:158[C]:PHE:HE2	2:N:163[C]:ALA:CA	2.21	0.49
1:A:69[A]:LYS:HB2	1:A:69[A]:LYS:HZ2	1.77	0.49
1:A:195[A]:SER:O	1:A:199[A]:ARG:HG3	2.12	0.49
1:E:406[A]:ILE:O	1:E:407[A]:LEU:HD23	2.13	0.49
1:G:256[A]:VAL:O	1:G:256[A]:VAL:CG2	2.59	0.49
1:H:308[A]:PHE:CZ	1:H:334[A]:GLU:HG2	2.48	0.49
2:L:159[A]:THR:O	2:L:162[A]:ASP:HB2	2.13	0.49
2:N:152[A]:THR:O	2:N:157[A]:ILE:O	2.31	0.49
1:A:69[C]:LYS:HB2	1:A:69[C]:LYS:HZ2	1.77	0.49
1:A:195[C]:SER:O	1:A:199[C]:ARG:HG3	2.12	0.49
1:E:406[C]:ILE:O	1:E:407[C]:LEU:HD23	2.13	0.49
1:G:256[C]:VAL:O	1:G:256[C]:VAL:CG2	2.59	0.49
1:H:308[C]:PHE:CZ	1:H:334[C]:GLU:HG2	2.48	0.49
2:K:130[C]:ARG:O	2:K:157[C]:ILE:CG2	2.56	0.49
1:B:43[A]:GLY:HA2	3:B:4751[A]:FAD:O3B	2.13	0.49
1:D:251[A]:ASP:OD1	1:D:253[A]:LYS:HG3	2.13	0.49
1:E:153[A]:THR:HB	1:E:278[A]:ILE:HG22	1.95	0.49
1:E:312[A]:ILE:HG21	1:E:315[A]:ILE:HD12	1.94	0.49
1:G:171[A]:ALA:CB	1:G:193[A]:LEU:HD23	2.42	0.49
1:I:226[A]:PHE:CZ	1:I:358[A]:ILE:HD11	2.47	0.49
1:I:353[A]:CYS:HB3	1:I:436[A]:LEU:CD2	2.38	0.49
2:N:168[A]:GLN:O	2:N:171[A]:GLN:CB	2.60	0.49
3:A:4751[C]:FAD:O3B	1:B:43[C]:GLY:HA2	2.13	0.49
1:D:251[C]:ASP:OD1	1:D:253[C]:LYS:HG3	2.13	0.49
1:E:153[C]:THR:HB	1:E:278[C]:ILE:HG22	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:312[C]:ILE:HG21	1:E:315[C]:ILE:HD12	1.94	0.49
1:G:171[C]:ALA:CB	1:G:193[C]:LEU:HD23	2.42	0.49
1:I:226[C]:PHE:CZ	1:I:358[C]:ILE:HD11	2.47	0.49
1:I:353[C]:CYS:HB3	1:I:436[C]:LEU:CD2	2.38	0.49
2:M:154[C]:PRO:O	2:M:155[C]:ARG:C	2.50	0.49
1:B:280[A]:ARG:HB2	1:B:326[A]:MET:HE1	1.94	0.49
1:B:454[A]:THR:N	1:B:457[A]:GLU:OE2	2.42	0.49
1:C:434[A]:LEU:HD23	1:C:434[A]:LEU:C	2.33	0.49
1:C:438[A]:TYR:CD1	2:L:157[A]:ILE:HD11	2.47	0.49
1:D:1[A]:ALA:CA	1:D:136[A]:THR:HG23	2.41	0.49
1:D:308[A]:PHE:O	1:D:316[A]:TYR:HB3	2.13	0.49
1:E:51[A]:ILE:HG23	1:F:396[A]:THR:HG21	1.94	0.49
1:G:133[A]:ASP:CG	1:G:134[A]:GLY:N	2.66	0.49
1:H:160[A]:ILE:HD13	1:H:167[A]:SER:HB3	1.95	0.49
1:I:225[A]:ASN:HD22	1:I:228[A]:ARG:HH12	1.60	0.49
1:I:383[A]:VAL:O	1:I:383[A]:VAL:HG13	2.13	0.49
1:J:37[A]:LYS:NZ	4:J:4759[A]:FAD:O2B	2.32	0.49
1:J:43[A]:GLY:HA2	4:J:4759[A]:FAD:O3B	2.12	0.49
1:J:59[A]:ASN:HD22	1:J:59[A]:ASN:N	2.11	0.49
1:J:437[A]:GLU:O	2:O:136[A]:ARG:NH2	2.46	0.49
1:B:280[C]:ARG:HB2	1:B:326[C]:MET:HE1	1.94	0.49
1:B:454[C]:THR:N	1:B:457[C]:GLU:OE2	2.42	0.49
1:C:434[C]:LEU:HD23	1:C:434[C]:LEU:C	2.33	0.49
1:D:1[C]:ALA:CA	1:D:136[C]:THR:HG23	2.41	0.49
1:D:308[C]:PHE:O	1:D:316[C]:TYR:HB3	2.13	0.49
1:E:51[C]:ILE:HG23	1:F:396[C]:THR:HG21	1.94	0.49
1:G:133[C]:ASP:CG	1:G:134[C]:GLY:N	2.66	0.49
1:H:160[C]:ILE:HD13	1:H:167[C]:SER:HB3	1.95	0.49
1:I:225[C]:ASN:HD22	1:I:228[C]:ARG:HH12	1.60	0.49
1:I:383[C]:VAL:O	1:I:383[C]:VAL:HG13	2.13	0.49
3:I:4759[C]:FAD:O2B	1:J:37[C]:LYS:NZ	2.32	0.49
3:I:4759[C]:FAD:O3B	1:J:43[C]:GLY:HA2	2.12	0.49
1:J:59[C]:ASN:HD22	1:J:59[C]:ASN:N	2.11	0.49
2:L:138[C]:ILE:O	2:L:138[C]:ILE:HG12	2.12	0.49
1:E:20[A]:VAL:HG23	1:E:336[A]:ILE:HD12	1.93	0.48
1:F:246[A]:ALA:HA	1:F:255[A]:ASP:O	2.12	0.48
1:I:49[A]:GLY:HA2	3:I:4758[A]:FAD:HM82	1.94	0.48
2:O:154[A]:PRO:C	2:O:156[A]:GLY:H	2.17	0.48
2:O:162[A]:ASP:HB3	2:O:165[A]:LYS:NZ	2.28	0.48
1:E:20[C]:VAL:HG23	1:E:336[C]:ILE:HD12	1.93	0.48
1:F:246[C]:ALA:HA	1:F:255[C]:ASP:O	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:4758[C]:FAD:HM82	1:I:49[C]:GLY:HA2	1.94	0.48
1:A:171[A]:ALA:HA	1:A:174[A]:LEU:CD2	2.43	0.48
1:B:148[A]:THR:O	3:B:4751[A]:FAD:H8A	2.13	0.48
1:D:133[A]:ASP:O	1:D:134[A]:GLY:C	2.52	0.48
1:F:84[A]:ASN:ND2	1:F:86[A]:ASP:HB2	2.28	0.48
1:G:74[A]:ARG:HE	1:H:59[A]:ASN:HD21	1.59	0.48
1:A:171[C]:ALA:HA	1:A:174[C]:LEU:CD2	2.43	0.48
3:A:4751[C]:FAD:H8A	1:B:148[C]:THR:O	2.13	0.48
1:D:133[C]:ASP:O	1:D:134[C]:GLY:C	2.52	0.48
1:F:84[C]:ASN:ND2	1:F:86[C]:ASP:HB2	2.28	0.48
1:G:74[C]:ARG:HE	1:H:59[C]:ASN:HD21	1.59	0.48
1:A:148[A]:THR:HG21	1:A:287[A]:LEU:HD21	1.96	0.48
1:B:189[A]:ILE:CG2	3:B:4751[A]:FAD:HM73	2.42	0.48
1:C:9[A]:VAL:HG21	1:C:342[A]:MET:CE	2.44	0.48
1:E:404[A]:VAL:HG22	1:E:420[A]:ILE:HG23	1.95	0.48
1:H:409[A]:GLN:CA	1:H:416[A]:LEU:HD11	2.44	0.48
1:J:280[A]:ARG:CG	1:J:280[A]:ARG:NH1	2.73	0.48
1:J:439[A]:GLY:O	1:J:440[A]:ALA:C	2.52	0.48
2:M:159[A]:THR:HB	2:M:162[A]:ASP:CG	2.34	0.48
1:A:148[C]:THR:HG21	1:A:287[C]:LEU:HD21	1.96	0.48
3:A:4751[C]:FAD:HM73	1:B:189[C]:ILE:CG2	2.42	0.48
1:C:9[C]:VAL:HG21	1:C:342[C]:MET:CE	2.44	0.48
1:E:404[C]:VAL:HG22	1:E:420[C]:ILE:HG23	1.95	0.48
1:H:409[C]:GLN:CA	1:H:416[C]:LEU:HD11	2.44	0.48
1:J:280[C]:ARG:CG	1:J:280[C]:ARG:NH1	2.73	0.48
1:J:439[C]:GLY:O	1:J:440[C]:ALA:C	2.52	0.48
2:L:151[C]:ALA:HB1	2:L:162[C]:ASP:CG	2.34	0.48
1:B:195[A]:SER:O	1:B:199[A]:ARG:HG3	2.12	0.48
1:B:395[A]:LYS:HD3	1:B:400[A]:THR:HG21	1.95	0.48
1:D:69[A]:LYS:NZ	1:D:73[A]:SER:HB3	2.28	0.48
1:F:160[A]:ILE:HA	1:F:165[A]:ILE:HG22	1.95	0.48
1:F:297[A]:ASP:HB2	1:F:298[A]:PRO:HD2	1.95	0.48
1:F:339[A]:VAL:HA	1:F:342[A]:MET:HG3	1.96	0.48
1:F:392[A]:SER:O	1:F:396[A]:THR:HG23	2.14	0.48
1:G:339[A]:VAL:CG1	1:G:342[A]:MET:HE3	2.26	0.48
1:I:24[A]:LYS:HB3	1:I:339[A]:VAL:HG21	1.95	0.48
1:I:25[A]:ALA:HB3	1:I:32[A]:THR:HG21	1.95	0.48
1:I:439[A]:GLY:O	1:I:440[A]:ALA:C	2.49	0.48
1:J:10[A]:THR:HG23	1:J:33[A]:VAL:HG12	1.96	0.48
2:K:161[A]:GLU:HA	2:K:164[A]:LEU:HD12	1.95	0.48
1:B:195[C]:SER:O	1:B:199[C]:ARG:HG3	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:395[C]:LYS:HD3	1:B:400[C]:THR:HG21	1.95	0.48
1:D:69[C]:LYS:NZ	1:D:73[C]:SER:HB3	2.28	0.48
1:F:160[C]:ILE:HA	1:F:165[C]:ILE:HG22	1.95	0.48
1:F:297[C]:ASP:HB2	1:F:298[C]:PRO:HD2	1.95	0.48
1:F:339[C]:VAL:HA	1:F:342[C]:MET:HG3	1.96	0.48
1:F:392[C]:SER:O	1:F:396[C]:THR:HG23	2.14	0.48
1:G:339[C]:VAL:CG1	1:G:342[C]:MET:HE3	2.26	0.48
1:I:24[C]:LYS:HB3	1:I:339[C]:VAL:HG21	1.95	0.48
1:I:25[C]:ALA:HB3	1:I:32[C]:THR:HG21	1.95	0.48
1:I:439[C]:GLY:O	1:I:440[C]:ALA:C	2.49	0.48
1:J:10[C]:THR:HG23	1:J:33[C]:VAL:HG12	1.96	0.48
1:D:44[A]:THR:O	1:D:45[A]:CYS:C	2.51	0.48
1:D:337[A]:ILE:HD13	1:D:349[A]:ILE:HB	1.95	0.48
1:D:445[A]:ILE:HG21	1:D:463[A]:ASN:ND2	2.28	0.48
1:F:443[A]:GLU:OE2	1:F:447[A]:ARG:NH1	2.46	0.48
1:G:119[A]:GLY:HA2	1:G:129[A]:ALA:HA	1.95	0.48
1:J:62[A]:TYR:HD1	1:J:65[A]:MET:HE2	1.77	0.48
1:D:44[C]:THR:O	1:D:45[C]:CYS:C	2.51	0.48
1:D:337[C]:ILE:HD13	1:D:349[C]:ILE:HB	1.95	0.48
1:D:445[C]:ILE:HG21	1:D:463[C]:ASN:ND2	2.28	0.48
1:F:443[C]:GLU:OE2	1:F:447[C]:ARG:NH1	2.46	0.48
1:G:119[C]:GLY:HA2	1:G:129[C]:ALA:HA	1.95	0.48
1:J:62[C]:TYR:HD1	1:J:65[C]:MET:HE2	1.77	0.48
1:A:382[A]:LYS:HE3	1:A:466[A]:ALA:O	2.13	0.48
1:B:290[A]:GLU:HB2	1:B:291[A]:GLU:OE2	2.12	0.48
1:B:388[A]:PHE:CE2	1:B:422[A]:GLY:HA3	2.49	0.48
1:B:406[A]:ILE:C	1:B:406[A]:ILE:CD1	2.78	0.48
1:B:461[A]:GLU:OE2	1:B:473[A]:ASN:HB2	2.13	0.48
1:C:330[A]:LYS:HD3	1:C:334[A]:GLU:OE2	2.14	0.48
1:D:284[A]:THR:O	1:D:284[A]:THR:CG2	2.60	0.48
1:D:290[A]:GLU:CD	1:D:290[A]:GLU:H	2.17	0.48
1:F:144[A]:ILE:HD11	1:F:146[A]:ILE:CD1	2.37	0.48
1:F:360[A]:THR:O	1:F:363[A]:GLU:HG2	2.13	0.48
1:F:368[A]:GLY:HA3	1:F:417[A]:GLY:HA2	1.95	0.48
1:G:133[A]:ASP:CG	1:G:134[A]:GLY:H	2.17	0.48
1:G:341[A]:GLY:HA2	1:G:345[A]:GLY:HA2	1.96	0.48
1:G:410[A]:LYS:CG	1:G:410[A]:LYS:O	2.61	0.48
2:M:139[A]:LEU:HD23	2:M:144[A]:LEU:HD12	1.95	0.48
1:A:382[C]:LYS:HE3	1:A:466[C]:ALA:O	2.13	0.48
1:B:290[C]:GLU:HB2	1:B:291[C]:GLU:OE2	2.12	0.48
1:B:388[C]:PHE:CE2	1:B:422[C]:GLY:HA3	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:406[C]:ILE:C	1:B:406[C]:ILE:CD1	2.78	0.48
1:B:461[C]:GLU:OE2	1:B:473[C]:ASN:HB2	2.13	0.48
1:C:330[C]:LYS:HD3	1:C:334[C]:GLU:OE2	2.14	0.48
1:D:284[C]:THR:O	1:D:284[C]:THR:CG2	2.60	0.48
1:D:290[C]:GLU:CD	1:D:290[C]:GLU:H	2.17	0.48
1:F:144[C]:ILE:HD11	1:F:146[C]:ILE:CD1	2.37	0.48
1:F:360[C]:THR:O	1:F:363[C]:GLU:HG2	2.13	0.48
1:F:368[C]:GLY:HA3	1:F:417[C]:GLY:HA2	1.95	0.48
1:G:133[C]:ASP:CG	1:G:134[C]:GLY:H	2.17	0.48
1:G:341[C]:GLY:HA2	1:G:345[C]:GLY:HA2	1.96	0.48
1:G:410[C]:LYS:CG	1:G:410[C]:LYS:O	2.61	0.48
1:H:412[C]:THR:HB	2:N:161[C]:GLU:HG3	1.96	0.48
1:A:358[A]:ILE:HD12	1:A:360[A]:THR:H	1.77	0.48
1:A:409[A]:GLN:HG2	1:A:412[A]:THR:OG1	2.13	0.48
1:B:45[A]:CYS:SG	1:B:50[A]:CYS:HB2	2.53	0.48
1:B:380[A]:GLU:HG3	1:J:84[A]:ASN:ND2	2.29	0.48
1:C:44[A]:THR:HG23	3:C:4752[A]:FAD:O2A	2.13	0.48
1:D:226[A]:PHE:CZ	1:D:230[A]:LEU:HD11	2.49	0.48
1:G:409[A]:GLN:HG3	1:G:412[A]:THR:H	1.79	0.48
1:J:389[A]:ALA:HA	1:J:400[A]:THR:HB	1.95	0.48
1:A:358[C]:ILE:HD12	1:A:360[C]:THR:H	1.77	0.48
1:A:409[C]:GLN:HG2	1:A:412[C]:THR:OG1	2.13	0.48
1:B:45[C]:CYS:SG	1:B:50[C]:CYS:HB2	2.53	0.48
1:B:380[C]:GLU:HG3	1:J:84[C]:ASN:ND2	2.29	0.48
3:B:4752[C]:FAD:O2A	1:C:44[C]:THR:HG23	2.13	0.48
1:D:226[C]:PHE:CZ	1:D:230[C]:LEU:HD11	2.49	0.48
1:G:409[C]:GLN:HG3	1:G:412[C]:THR:H	1.79	0.48
1:J:389[C]:ALA:HA	1:J:400[C]:THR:HB	1.95	0.48
1:C:9[A]:VAL:CG2	1:C:342[A]:MET:CE	2.86	0.48
1:C:332[A]:GLU:O	1:C:336[A]:ILE:HG13	2.14	0.48
1:E:49[A]:GLY:HA2	3:E:4754[A]:FAD:HM82	1.96	0.48
1:G:402[A]:GLY:HA3	1:G:421[A]:LEU:O	2.14	0.48
1:I:290[A]:GLU:C	1:I:292[A]:LEU:H	2.16	0.48
1:J:188[A]:VAL:HG11	4:J:4785[A]:HOH:O	2.14	0.48
2:M:164[A]:LEU:O	2:M:165[A]:LYS:C	2.52	0.48
1:C:9[C]:VAL:CG2	1:C:342[C]:MET:CE	2.86	0.48
1:C:332[C]:GLU:O	1:C:336[C]:ILE:HG13	2.14	0.48
3:D:4754[C]:FAD:HM82	1:E:49[C]:GLY:HA2	1.96	0.48
1:G:402[C]:GLY:HA3	1:G:421[C]:LEU:O	2.14	0.48
1:I:290[C]:GLU:C	1:I:292[C]:LEU:H	2.16	0.48
4:I:4786[C]:HOH:O	1:J:188[C]:VAL:HG11	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:138[C]:ILE:CD1	2:L:163[C]:ALA:O	2.62	0.48
2:L:142[C]:HIS:HB2	2:L:144[C]:LEU:CD2	2.43	0.48
2:N:130[C]:ARG:O	2:N:157[C]:ILE:CG2	2.59	0.48
1:E:366[A]:TRP:CB	1:E:419[A]:HIS:HD2	2.26	0.48
1:G:186[A]:ALA:HB1	1:G:213[A]:VAL:HG13	1.95	0.48
1:J:155[A]:PHE:HZ	1:J:243[A]:VAL:HG22	1.79	0.48
2:K:159[A]:THR:HB	2:K:162[A]:ASP:OD1	2.14	0.48
1:E:366[C]:TRP:CB	1:E:419[C]:HIS:HD2	2.26	0.48
1:G:186[C]:ALA:HB1	1:G:213[C]:VAL:HG13	1.95	0.48
1:J:155[C]:PHE:HZ	1:J:243[C]:VAL:HG22	1.79	0.48
2:L:135[C]:ALA:HB2	2:L:158[C]:PHE:O	2.14	0.48
1:A:59[A]:ASN:ND2	1:A:91[A]:GLN:OE1	2.46	0.48
1:A:177[A]:VAL:HG22	1:A:197[A]:TRP:CE3	2.49	0.48
1:B:258[A]:ILE:O	1:B:259[A]:GLU:HB2	2.13	0.48
1:D:162[A]:GLU:OE1	1:D:162[A]:GLU:CA	2.56	0.48
1:D:250[A]:SER:HB3	1:G:304[A]:VAL:HG23	1.95	0.48
1:H:178[A]:PRO:HB3	1:H:273[A]:VAL:HG21	1.96	0.48
2:L:170[A]:LYS:HD3	2:L:170[A]:LYS:C	2.33	0.48
1:A:59[C]:ASN:ND2	1:A:91[C]:GLN:OE1	2.46	0.48
1:A:177[C]:VAL:HG22	1:A:197[C]:TRP:CE3	2.49	0.48
1:B:258[C]:ILE:O	1:B:259[C]:GLU:HB2	2.13	0.48
1:D:162[C]:GLU:OE1	1:D:162[C]:GLU:CA	2.56	0.48
1:D:250[C]:SER:HB3	1:G:304[C]:VAL:HG23	1.95	0.48
1:H:178[C]:PRO:HB3	1:H:273[C]:VAL:HG21	1.96	0.48
1:A:155[A]:PHE:HZ	1:A:243[A]:VAL:HG22	1.78	0.47
1:D:305[A]:ASN:HD21	1:D:309[A]:GLN:H	1.61	0.47
1:F:1[A]:ALA:H3	1:F:136[A]:THR:HG22	1.78	0.47
1:G:84[A]:ASN:HD21	1:G:86[A]:ASP:HB2	1.79	0.47
1:H:389[A]:ALA:HA	1:H:400[A]:THR:CG2	2.44	0.47
1:I:438[A]:TYR:OH	1:J:440[A]:ALA:CB	2.62	0.47
1:J:71[A]:PHE:HA	1:J:74[A]:ARG:HG3	1.96	0.47
2:O:149[A]:GLY:N	2:O:166[A]:LEU:HD11	2.20	0.47
1:A:155[C]:PHE:HZ	1:A:243[C]:VAL:HG22	1.78	0.47
1:D:305[C]:ASN:HD21	1:D:309[C]:GLN:H	1.61	0.47
1:F:1[C]:ALA:H3	1:F:136[C]:THR:HG22	1.78	0.47
1:G:84[C]:ASN:HD21	1:G:86[C]:ASP:HB2	1.79	0.47
1:H:389[C]:ALA:HA	1:H:400[C]:THR:CG2	2.44	0.47
1:I:438[C]:TYR:OH	1:J:440[C]:ALA:CB	2.62	0.47
1:J:71[C]:PHE:HA	1:J:74[C]:ARG:HG3	1.96	0.47
1:B:137[A]:GLN:HE21	1:B:137[A]:GLN:HA	1.75	0.47
1:D:297[A]:ASP:OD1	1:D:301[A]:ARG:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:224[A]:LYS:HA	1:I:224[A]:LYS:HD2	1.78	0.47
1:J:69[A]:LYS:HB2	1:J:69[A]:LYS:HZ2	1.79	0.47
1:J:308[A]:PHE:CZ	1:J:334[A]:GLU:HG2	2.49	0.47
1:J:468[A]:PHE:CD2	1:J:470[A]:LYS:NZ	2.76	0.47
1:B:137[C]:GLN:HE21	1:B:137[C]:GLN:HA	1.75	0.47
1:B:438[C]:TYR:HE1	2:K:157[C]:ILE:HD11	1.79	0.47
1:D:297[C]:ASP:OD1	1:D:301[C]:ARG:HB2	2.14	0.47
1:I:224[C]:LYS:HA	1:I:224[C]:LYS:HD2	1.78	0.47
1:J:69[C]:LYS:HB2	1:J:69[C]:LYS:HZ2	1.79	0.47
1:J:308[C]:PHE:CZ	1:J:334[C]:GLU:HG2	2.49	0.47
1:J:468[C]:PHE:CD2	1:J:470[C]:LYS:NZ	2.76	0.47
1:B:6[A]:ASP:O	1:B:31[A]:LYS:HD3	2.15	0.47
1:C:145[A]:LEU:HD21	1:C:318[A]:ILE:HG23	1.96	0.47
1:D:383[A]:VAL:HB	1:D:407[A]:LEU:HD23	1.96	0.47
1:F:91[A]:GLN:HG3	1:F:92[A]:LYS:N	2.28	0.47
1:G:347[A]:VAL:O	1:G:347[A]:VAL:CG2	2.62	0.47
1:H:285[A]:LYS:HB2	4:H:4820[A]:HOH:O	2.14	0.47
1:I:184[A]:ILE:CD1	1:I:274[A]:LEU:HD11	2.43	0.47
1:I:320[A]:ASP:OD1	3:I:4758[A]:FAD:H5'2	2.13	0.47
1:J:67[A]:HIS:CA	1:J:81[A]:VAL:HG11	2.36	0.47
1:J:473[A]:ASN:OD1	4:J:4771[A]:HOH:O	2.20	0.47
2:O:150[A]:THR:HG22	2:O:151[A]:ALA:N	2.29	0.47
1:B:6[C]:ASP:O	1:B:31[C]:LYS:HD3	2.15	0.47
1:C:145[C]:LEU:HD21	1:C:318[C]:ILE:HG23	1.96	0.47
1:D:383[C]:VAL:HB	1:D:407[C]:LEU:HD23	1.96	0.47
1:F:91[C]:GLN:HG3	1:F:92[C]:LYS:N	2.28	0.47
1:G:347[C]:VAL:O	1:G:347[C]:VAL:CG2	2.62	0.47
4:G:4820[C]:HOH:O	1:H:285[C]:LYS:HB2	2.14	0.47
3:H:4758[C]:FAD:H5'2	1:I:320[C]:ASP:OD1	2.13	0.47
1:I:184[C]:ILE:CD1	1:I:274[C]:LEU:HD11	2.43	0.47
4:I:4772[C]:HOH:O	1:J:473[C]:ASN:OD1	2.20	0.47
1:J:67[C]:HIS:CA	1:J:81[C]:VAL:HG11	2.36	0.47
2:M:145[C]:ASP:H	2:M:148[C]:GLN:HE21	1.62	0.47
1:B:46[A]:LEU:HD12	1:B:46[A]:LEU:C	2.28	0.47
1:B:386[A]:PHE:HA	1:B:387[A]:PRO:HD3	1.68	0.47
1:C:59[A]:ASN:ND2	1:D:74[A]:ARG:HE	2.13	0.47
1:J:194[A]:GLY:O	1:J:198[A]:GLN:HB2	2.15	0.47
1:B:46[C]:LEU:HD12	1:B:46[C]:LEU:C	2.28	0.47
1:B:386[C]:PHE:HA	1:B:387[C]:PRO:HD3	1.68	0.47
1:C:59[C]:ASN:ND2	1:D:74[C]:ARG:HE	2.13	0.47
1:J:194[C]:GLY:O	1:J:198[C]:GLN:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326[A]:MET:HE2	4:A:4777[A]:HOH:O	2.14	0.47
1:B:131[A]:LYS:HG3	1:B:135[A]:GLY:O	2.15	0.47
1:D:97[A]:LYS:O	1:D:100[A]:THR:HG22	2.14	0.47
1:F:382[A]:LYS:NZ	1:F:413[A]:ASP:OD1	2.29	0.47
1:G:299[A]:ARG:HG2	1:G:301[A]:ARG:HG3	1.96	0.47
1:H:433[A]:ALA:O	1:H:437[A]:GLU:HG2	2.13	0.47
1:I:230[A]:LEU:HD12	1:I:230[A]:LEU:HA	1.76	0.47
1:I:287[A]:LEU:HB3	1:I:289[A]:LEU:HG	1.95	0.47
1:I:296[A]:LEU:C	1:I:297[A]:ASP:O	2.52	0.47
1:I:404[A]:VAL:HG11	1:I:459[A]:PHE:HA	1.96	0.47
1:A:326[C]:MET:HE2	4:J:4777[C]:HOH:O	2.14	0.47
1:B:131[C]:LYS:HG3	1:B:135[C]:GLY:O	2.15	0.47
1:D:97[C]:LYS:O	1:D:100[C]:THR:HG22	2.14	0.47
1:F:382[C]:LYS:NZ	1:F:413[C]:ASP:OD1	2.29	0.47
1:G:299[C]:ARG:HG2	1:G:301[C]:ARG:HG3	1.96	0.47
1:H:433[C]:ALA:O	1:H:437[C]:GLU:HG2	2.13	0.47
1:I:230[C]:LEU:HD12	1:I:230[C]:LEU:HA	1.76	0.47
1:I:287[C]:LEU:HB3	1:I:289[C]:LEU:HG	1.95	0.47
1:I:296[C]:LEU:C	1:I:297[C]:ASP:O	2.52	0.47
1:I:404[C]:VAL:HG11	1:I:459[C]:PHE:HA	1.96	0.47
1:A:184[A]:ILE:CD1	1:A:274[A]:LEU:HD11	2.44	0.47
1:C:303[A]:PRO:C	1:C:304[A]:VAL:HG13	2.35	0.47
1:C:389[A]:ALA:HA	1:C:400[A]:THR:HB	1.97	0.47
1:C:409[A]:GLN:HG3	1:C:412[A]:THR:H	1.79	0.47
1:D:354[A]:VAL:HA	1:D:355[A]:PRO:HD3	1.70	0.47
1:G:307[A]:ARG:O	1:G:308[A]:PHE:HB2	2.15	0.47
1:H:406[A]:ILE:C	1:H:406[A]:ILE:HD12	2.34	0.47
1:A:184[C]:ILE:CD1	1:A:274[C]:LEU:HD11	2.44	0.47
1:C:303[C]:PRO:C	1:C:304[C]:VAL:HG13	2.35	0.47
1:C:389[C]:ALA:HA	1:C:400[C]:THR:HB	1.97	0.47
1:C:409[C]:GLN:HG3	1:C:412[C]:THR:H	1.79	0.47
1:D:354[C]:VAL:HA	1:D:355[C]:PRO:HD3	1.70	0.47
1:G:307[C]:ARG:O	1:G:308[C]:PHE:HB2	2.15	0.47
1:H:406[C]:ILE:C	1:H:406[C]:ILE:HD12	2.34	0.47
2:N:131[C]:LEU:CD2	2:N:146[C]:ALA:HB1	2.44	0.47
1:A:265[A]:LYS:O	1:A:266[A]:ALA:C	2.53	0.47
1:B:2[A]:ASP:HB3	1:B:136[A]:THR:O	2.15	0.47
1:B:308[A]:PHE:CZ	1:B:334[A]:GLU:HG2	2.49	0.47
1:C:46[A]:LEU:HD21	1:C:100[A]:THR:N	2.30	0.47
1:D:8[A]:ASP:OD1	1:D:31[A]:LYS:O	2.31	0.47
1:D:54[A]:LYS:N	1:D:54[A]:LYS:HE3	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:182[A]:VAL:HG22	1:E:274[A]:LEU:CD1	2.44	0.47
1:E:307[A]:ARG:HA	1:E:347[A]:VAL:HG21	1.96	0.47
1:F:346[A]:ALA:CB	2:M:140[A]:GLU:HB3	2.45	0.47
1:G:106[A]:LEU:HD11	1:H:473[A]:ASN:HA	1.95	0.47
1:G:110[A]:ASN:C	1:G:111[A]:LYS:CG	2.82	0.47
1:G:393[A]:ARG:NH1	1:G:454[A]:THR:HA	2.30	0.47
1:H:468[A]:PHE:CG	1:H:469[A]:GLY:N	2.83	0.47
1:I:33[A]:VAL:HB	1:I:113[A]:VAL:HG23	1.97	0.47
1:I:99[A]:LEU:HD23	1:I:99[A]:LEU:HA	1.53	0.47
2:K:131[A]:LEU:HD12	2:K:158[A]:PHE:HB3	1.96	0.47
2:L:131[A]:LEU:O	2:L:157[A]:ILE:HG21	2.14	0.47
2:N:158[A]:PHE:CE2	2:N:163[A]:ALA:N	2.83	0.47
1:A:265[C]:LYS:O	1:A:266[C]:ALA:C	2.53	0.47
1:B:2[C]:ASP:HB3	1:B:136[C]:THR:O	2.15	0.47
1:B:308[C]:PHE:CZ	1:B:334[C]:GLU:HG2	2.49	0.47
1:C:46[C]:LEU:HD21	1:C:100[C]:THR:N	2.30	0.47
1:D:8[C]:ASP:OD1	1:D:31[C]:LYS:O	2.31	0.47
1:D:54[C]:LYS:N	1:D:54[C]:LYS:HE3	2.30	0.47
1:E:182[C]:VAL:HG22	1:E:274[C]:LEU:CD1	2.44	0.47
1:E:307[C]:ARG:HA	1:E:347[C]:VAL:HG21	1.96	0.47
1:G:106[C]:LEU:HD11	1:H:473[C]:ASN:HA	1.95	0.47
1:G:110[C]:ASN:C	1:G:111[C]:LYS:CG	2.82	0.47
1:G:393[C]:ARG:NH1	1:G:454[C]:THR:HA	2.30	0.47
1:H:468[C]:PHE:CG	1:H:469[C]:GLY:N	2.83	0.47
1:I:33[C]:VAL:HB	1:I:113[C]:VAL:HG23	1.97	0.47
1:I:99[C]:LEU:HD23	1:I:99[C]:LEU:HA	1.53	0.47
2:K:139[C]:LEU:HG	2:K:158[C]:PHE:HE2	1.79	0.47
2:L:142[C]:HIS:HB2	2:L:144[C]:LEU:HD22	1.96	0.47
2:M:146[C]:ALA:C	2:M:148[C]:GLN:N	2.67	0.47
2:N:135[C]:ALA:CB	2:N:163[C]:ALA:HB2	2.45	0.47
1:B:184[A]:ILE:HD13	1:B:243[A]:VAL:HG11	1.96	0.47
1:C:445[A]:ILE:HG21	1:C:463[A]:ASN:OD1	2.14	0.47
1:E:57[A]:LEU:HD11	1:E:192[A]:GLU:HB3	1.97	0.47
1:F:452[A]:HIS:HA	1:F:453[A]:PRO:HA	1.73	0.47
1:I:214[A]:GLY:HA3	1:I:218[A]:ILE:HG13	1.96	0.47
1:J:406[A]:ILE:O	1:J:407[A]:LEU:HD23	2.15	0.47
2:O:155[A]:ARG:N	2:O:157[A]:ILE:CD1	2.77	0.47
2:O:159[A]:THR:OG1	2:O:161[A]:GLU:HB2	2.15	0.47
1:B:184[C]:ILE:HD13	1:B:243[C]:VAL:HG11	1.96	0.47
1:C:445[C]:ILE:HG21	1:C:463[C]:ASN:OD1	2.14	0.47
1:E:57[C]:LEU:HD11	1:E:192[C]:GLU:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:452[C]:HIS:HA	1:F:453[C]:PRO:HA	1.73	0.47
1:I:214[C]:GLY:HA3	1:I:218[C]:ILE:HG13	1.96	0.47
1:J:406[C]:ILE:O	1:J:407[C]:LEU:HD23	2.15	0.47
1:A:70[A]:ASP:OD1	1:A:74[A]:ARG:HD2	2.13	0.47
1:I:320[A]:ASP:HB3	1:I:326[A]:MET:HE1	1.97	0.47
1:J:144[A]:ILE:C	1:J:144[A]:ILE:HD12	2.35	0.47
1:J:174[A]:LEU:HD22	1:J:197[A]:TRP:CE2	2.50	0.47
1:A:70[C]:ASP:OD1	1:A:74[C]:ARG:HD2	2.13	0.47
1:I:320[C]:ASP:HB3	1:I:326[C]:MET:HE1	1.97	0.47
1:J:144[C]:ILE:C	1:J:144[C]:ILE:HD12	2.35	0.47
1:J:174[C]:LEU:HD22	1:J:197[C]:TRP:CE2	2.50	0.47
1:B:164[A]:THR:CG2	1:B:248[A]:LYS:HZ2	2.28	0.47
1:C:326[A]:MET:CE	1:C:326[A]:MET:HB2	2.45	0.47
1:C:330[A]:LYS:HD2	1:C:330[A]:LYS:C	2.34	0.47
1:D:10[A]:THR:HG21	1:D:139[A]:ILE:CG2	2.44	0.47
1:F:154[A]:PRO:HD2	1:F:281[A]:ARG:NH2	2.30	0.47
1:B:164[C]:THR:CG2	1:B:248[C]:LYS:HZ2	2.28	0.47
1:C:326[C]:MET:CE	1:C:326[C]:MET:HB2	2.45	0.47
1:C:330[C]:LYS:HD2	1:C:330[C]:LYS:C	2.34	0.47
1:D:10[C]:THR:HG21	1:D:139[C]:ILE:CG2	2.44	0.47
1:F:154[C]:PRO:HD2	1:F:281[C]:ARG:NH2	2.30	0.47
2:N:152[C]:THR:O	2:N:157[C]:ILE:O	2.33	0.47
1:C:63[A]:TYR:HA	1:D:76[A]:ILE:HD13	1.96	0.46
1:E:450[A]:HIS:HA	1:F:430[A]:ASN:ND2	2.30	0.46
1:H:193[A]:LEU:HD12	1:H:193[A]:LEU:HA	1.64	0.46
1:I:88[A]:MET:CE	1:I:200[A]:LEU:HD11	2.44	0.46
1:I:155[A]:PHE:CD2	1:I:158[A]:ILE:HG13	2.49	0.46
1:C:63[C]:TYR:HA	1:D:76[C]:ILE:HD13	1.96	0.46
1:E:450[C]:HIS:HA	1:F:430[C]:ASN:ND2	2.30	0.46
1:H:193[C]:LEU:HD12	1:H:193[C]:LEU:HA	1.64	0.46
1:I:88[C]:MET:CE	1:I:200[C]:LEU:HD11	2.44	0.46
1:I:155[C]:PHE:CD2	1:I:158[C]:ILE:HG13	2.49	0.46
1:A:45[A]:CYS:SG	1:A:50[A]:CYS:HB2	2.53	0.46
1:A:69[A]:LYS:O	1:A:73[A]:SER:HB3	2.14	0.46
1:A:427[A]:GLU:OE2	1:B:455[A]:LEU:N	2.48	0.46
1:B:57[A]:LEU:HD11	1:B:192[A]:GLU:HG2	1.97	0.46
1:D:450[A]:HIS:HD2	1:D:460[A]:ARG:HG3	1.80	0.46
1:G:110[A]:ASN:C	1:G:111[A]:LYS:HG3	2.36	0.46
1:A:45[C]:CYS:SG	1:A:50[C]:CYS:HB2	2.53	0.46
1:A:69[C]:LYS:O	1:A:73[C]:SER:HB3	2.14	0.46
1:A:427[C]:GLU:OE2	1:B:455[C]:LEU:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:57[C]:LEU:HD11	1:B:192[C]:GLU:HG2	1.97	0.46
1:D:450[C]:HIS:HD2	1:D:460[C]:ARG:HG3	1.80	0.46
1:G:110[C]:ASN:C	1:G:111[C]:LYS:HG3	2.36	0.46
2:L:136[C]:ARG:O	2:L:139[C]:LEU:HB2	2.16	0.46
2:L:138[C]:ILE:HD11	2:L:163[C]:ALA:O	2.14	0.46
2:M:157[C]:ILE:HG22	2:M:158[C]:PHE:H	1.79	0.46
1:C:435[A]:ALA:HB1	1:C:445[A]:ILE:HD11	1.96	0.46
1:G:452[A]:HIS:HA	1:G:457[A]:GLU:OE2	2.15	0.46
1:C:435[C]:ALA:HB1	1:C:445[C]:ILE:HD11	1.96	0.46
1:G:452[C]:HIS:HA	1:G:457[C]:GLU:OE2	2.15	0.46
1:A:52[A]:PRO:HB2	1:A:172[A]:LEU:HD13	1.96	0.46
1:A:69[A]:LYS:NZ	1:A:69[A]:LYS:CB	2.79	0.46
1:C:164[A]:THR:HB	1:C:254[A]:ILE:HD11	1.97	0.46
1:D:46[A]:LEU:HD12	1:D:46[A]:LEU:O	2.15	0.46
1:E:180[A]:LYS:HD2	1:E:181[A]:MET:N	2.30	0.46
1:E:322[A]:VAL:HG12	1:E:323[A]:ALA:N	2.31	0.46
1:F:17[A]:GLY:HA2	1:F:332[A]:GLU:HA	1.97	0.46
1:F:404[A]:VAL:HG21	1:F:428[A]:MET:HE3	1.97	0.46
1:F:472[A]:ILE:N	1:F:472[A]:ILE:CD1	2.76	0.46
1:I:20[A]:VAL:HG23	1:I:336[A]:ILE:HD12	1.97	0.46
1:I:121[A]:ILE:HA	1:I:127[A]:VAL:HG12	1.97	0.46
1:I:428[A]:MET:HE1	1:I:456[A]:SER:N	2.30	0.46
1:I:428[A]:MET:CE	1:I:455[A]:LEU:HB3	2.45	0.46
1:J:124[A]:LYS:HB2	1:J:124[A]:LYS:HE3	1.49	0.46
1:A:52[C]:PRO:HB2	1:A:172[C]:LEU:HD13	1.96	0.46
1:A:69[C]:LYS:NZ	1:A:69[C]:LYS:CB	2.79	0.46
1:C:164[C]:THR:HB	1:C:254[C]:ILE:HD11	1.97	0.46
1:D:46[C]:LEU:O	1:D:46[C]:LEU:HD12	2.15	0.46
1:E:180[C]:LYS:HD2	1:E:181[C]:MET:N	2.30	0.46
1:E:322[C]:VAL:HG12	1:E:323[C]:ALA:N	2.31	0.46
1:F:17[C]:GLY:HA2	1:F:332[C]:GLU:HA	1.97	0.46
1:F:404[C]:VAL:HG21	1:F:428[C]:MET:HE3	1.97	0.46
1:F:472[C]:ILE:N	1:F:472[C]:ILE:CD1	2.76	0.46
1:I:20[C]:VAL:HG23	1:I:336[C]:ILE:HD12	1.97	0.46
1:I:121[C]:ILE:HA	1:I:127[C]:VAL:HG12	1.97	0.46
1:I:428[C]:MET:HE1	1:I:456[C]:SER:N	2.30	0.46
1:I:428[C]:MET:CE	1:I:455[C]:LEU:HB3	2.45	0.46
1:J:124[C]:LYS:HB2	1:J:124[C]:LYS:HE3	1.49	0.46
2:N:152[C]:THR:HG22	2:N:153[C]:GLY:N	2.29	0.46
1:A:79[A]:SER:HB2	1:B:79[A]:SER:HB3	1.96	0.46
1:A:168[A]:SER:OG	1:A:169[A]:THR:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:160[A]:ILE:HD11	1:B:276[A]:VAL:HB	1.98	0.46
1:B:432[A]:ALA:O	1:B:436[A]:LEU:CD2	2.62	0.46
1:E:199[A]:ARG:NH2	1:E:361[A]:HIS:H	2.13	0.46
1:E:434[A]:LEU:HD13	1:F:448[A]:VAL:HG21	1.98	0.46
1:I:14[A]:SER:HB3	1:I:42[A]:GLY:N	2.21	0.46
1:I:297[A]:ASP:HB3	1:I:299[A]:ARG:N	2.29	0.46
1:J:214[A]:GLY:HA3	1:J:218[A]:ILE:HD13	1.98	0.46
2:M:131[A]:LEU:HD13	2:M:136[A]:ARG:CZ	2.43	0.46
1:A:79[C]:SER:HB2	1:B:79[C]:SER:HB3	1.96	0.46
1:A:168[C]:SER:OG	1:A:169[C]:THR:N	2.48	0.46
1:B:160[C]:ILE:HD11	1:B:276[C]:VAL:HB	1.98	0.46
1:B:432[C]:ALA:O	1:B:436[C]:LEU:CD2	2.62	0.46
1:E:199[C]:ARG:NH2	1:E:361[C]:HIS:H	2.13	0.46
1:E:434[C]:LEU:HD13	1:F:448[C]:VAL:HG21	1.98	0.46
1:I:14[C]:SER:HB3	1:I:42[C]:GLY:N	2.21	0.46
1:I:297[C]:ASP:HB3	1:I:299[C]:ARG:N	2.29	0.46
1:J:214[C]:GLY:HA3	1:J:218[C]:ILE:HD13	1.98	0.46
2:K:131[C]:LEU:HG	2:K:136[C]:ARG:HB2	1.96	0.46
3:B:4751[A]:FAD:O4'	3:B:4751[A]:FAD:O2'	2.16	0.46
1:D:165[A]:ILE:HD13	1:D:165[A]:ILE:N	2.30	0.46
1:D:307[A]:ARG:O	1:D:308[A]:PHE:CB	2.54	0.46
1:E:339[A]:VAL:HG23	1:E:340[A]:GLU:N	2.30	0.46
1:F:15[A]:GLY:CA	1:F:43[A]:GLY:HA3	2.46	0.46
1:F:409[A]:GLN:HG2	1:F:412[A]:THR:HG23	1.97	0.46
1:H:175[A]:LYS:HD3	1:H:175[A]:LYS:HA	1.52	0.46
2:N:158[A]:PHE:HE2	2:N:163[A]:ALA:HB2	1.80	0.46
2:N:158[A]:PHE:CZ	2:N:163[A]:ALA:N	2.83	0.46
3:A:4751[C]:FAD:O4'	3:A:4751[C]:FAD:O2'	2.16	0.46
1:D:165[C]:ILE:HD13	1:D:165[C]:ILE:N	2.30	0.46
1:D:307[C]:ARG:O	1:D:308[C]:PHE:CB	2.54	0.46
1:E:339[C]:VAL:HG23	1:E:340[C]:GLU:N	2.30	0.46
1:F:15[C]:GLY:CA	1:F:43[C]:GLY:HA3	2.46	0.46
1:F:409[C]:GLN:HG2	1:F:412[C]:THR:HG23	1.97	0.46
1:H:175[C]:LYS:HD3	1:H:175[C]:LYS:HA	1.52	0.46
2:L:132[C]:SER:CB	2:L:135[C]:ALA:CB	2.94	0.46
1:B:41[A]:LEU:HD21	1:B:114[A]:HIS:NE2	2.31	0.46
1:C:53[A]:SER:HB3	1:C:54[A]:LYS:NZ	2.30	0.46
1:C:351[A]:TYR:O	1:C:354[A]:VAL:HG12	2.16	0.46
1:C:358[A]:ILE:HD11	1:C:360[A]:THR:HG23	1.98	0.46
1:C:393[A]:ARG:NH1	1:D:427[A]:GLU:OE2	2.49	0.46
1:C:473[A]:ASN:HA	1:D:106[A]:LEU:CD2	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:447[A]:ARG:HA	1:E:447[A]:ARG:HD3	1.55	0.46
1:G:56[A]:LEU:HA	1:G:56[A]:LEU:HD12	1.47	0.46
1:H:371[A]:GLU:OE2	1:H:405[A]:LYS:HE3	2.16	0.46
1:I:52[A]:PRO:HB2	1:I:172[A]:LEU:HD13	1.98	0.46
1:I:63[A]:TYR:CA	1:J:76[A]:ILE:HD13	2.46	0.46
1:I:122[A]:THR:OG1	1:I:126[A]:GLN:NE2	2.49	0.46
1:I:333[A]:ASP:O	1:I:334[A]:GLU:C	2.54	0.46
2:M:131[A]:LEU:CD1	2:M:136[A]:ARG:CZ	2.93	0.46
1:B:41[C]:LEU:HD21	1:B:114[C]:HIS:NE2	2.31	0.46
1:C:53[C]:SER:HB3	1:C:54[C]:LYS:NZ	2.30	0.46
1:C:351[C]:TYR:O	1:C:354[C]:VAL:HG12	2.16	0.46
1:C:358[C]:ILE:HD11	1:C:360[C]:THR:HG23	1.98	0.46
1:C:393[C]:ARG:NH1	1:D:427[C]:GLU:OE2	2.49	0.46
1:C:473[C]:ASN:HA	1:D:106[C]:LEU:CD2	2.45	0.46
1:E:447[C]:ARG:HD3	1:E:447[C]:ARG:HA	1.55	0.46
1:F:45[C]:CYS:SG	1:F:50[C]:CYS:SG	2.80	0.46
1:G:56[C]:LEU:HA	1:G:56[C]:LEU:HD12	1.47	0.46
1:H:371[C]:GLU:OE2	1:H:405[C]:LYS:HE3	2.16	0.46
1:I:52[C]:PRO:HB2	1:I:172[C]:LEU:HD13	1.98	0.46
1:I:63[C]:TYR:CA	1:J:76[C]:ILE:HD13	2.46	0.46
1:I:122[C]:THR:OG1	1:I:126[C]:GLN:NE2	2.49	0.46
1:I:333[C]:ASP:O	1:I:334[C]:GLU:C	2.54	0.46
1:A:200[A]:LEU:HA	1:A:200[A]:LEU:HD12	1.63	0.46
1:D:256[A]:VAL:HG22	1:D:269[A]:ILE:O	2.15	0.46
1:D:308[A]:PHE:CZ	1:D:334[A]:GLU:HG2	2.50	0.46
1:D:311[A]:LYS:HA	1:D:311[A]:LYS:HD3	1.82	0.46
1:E:251[A]:ASP:OD1	1:E:253[A]:LYS:HB2	2.16	0.46
1:F:172[A]:LEU:HD13	1:F:193[A]:LEU:HD21	1.97	0.46
1:G:472[A]:ILE:HD13	1:G:473[A]:ASN:N	2.31	0.46
1:I:41[A]:LEU:CD1	1:I:41[A]:LEU:N	2.73	0.46
1:I:305[A]:ASN:O	1:I:308[A]:PHE:N	2.45	0.46
2:L:142[A]:HIS:N	2:L:142[A]:HIS:ND1	2.64	0.46
1:A:200[C]:LEU:HA	1:A:200[C]:LEU:HD12	1.63	0.46
1:D:256[C]:VAL:HG22	1:D:269[C]:ILE:O	2.15	0.46
1:D:308[C]:PHE:CZ	1:D:334[C]:GLU:HG2	2.50	0.46
1:D:311[C]:LYS:HA	1:D:311[C]:LYS:HD3	1.82	0.46
1:E:251[C]:ASP:OD1	1:E:253[C]:LYS:HB2	2.16	0.46
1:F:172[C]:LEU:HD13	1:F:193[C]:LEU:HD21	1.97	0.46
1:G:472[C]:ILE:HD13	1:G:473[C]:ASN:N	2.31	0.46
1:I:41[C]:LEU:CD1	1:I:41[C]:LEU:N	2.73	0.46
1:I:305[C]:ASN:O	1:I:308[C]:PHE:N	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:159[C]:THR:HG21	2:K:161[C]:GLU:OE2	2.16	0.46
2:L:134[C]:ALA:O	2:L:138[C]:ILE:CG2	2.54	0.46
1:C:54[A]:LYS:HA	1:C:57[A]:LEU:HD12	1.96	0.46
1:G:49[A]:GLY:O	1:G:53[A]:SER:HB3	2.16	0.46
2:N:132[A]:SER:O	2:N:133[A]:PRO:C	2.54	0.46
2:O:150[A]:THR:HG22	2:O:151[A]:ALA:H	1.81	0.46
1:C:54[C]:LYS:HA	1:C:57[C]:LEU:HD12	1.96	0.46
1:D:412[C]:THR:HB	2:L:161[C]:GLU:CG	2.40	0.46
1:G:49[C]:GLY:O	1:G:53[C]:SER:HB3	2.16	0.46
2:L:132[C]:SER:H	2:L:135[C]:ALA:HB3	1.81	0.46
1:A:145[A]:LEU:HD21	1:A:318[A]:ILE:HG12	1.98	0.46
1:B:9[A]:VAL:HG22	1:B:32[A]:THR:HB	1.98	0.46
1:C:155[A]:PHE:CD1	1:C:158[A]:ILE:HD13	2.51	0.46
1:F:297[A]:ASP:O	1:F:298[A]:PRO:C	2.54	0.46
1:H:54[A]:LYS:NZ	1:H:192[A]:GLU:OE1	2.48	0.46
1:J:407[A]:LEU:HD23	1:J:407[A]:LEU:N	2.31	0.46
2:K:137[A]:ASN:ND2	2:K:138[A]:ILE:HG23	2.30	0.46
1:A:145[C]:LEU:HD21	1:A:318[C]:ILE:HG12	1.98	0.46
1:B:9[C]:VAL:HG22	1:B:32[C]:THR:HB	1.98	0.46
1:C:155[C]:PHE:CD1	1:C:158[C]:ILE:HD13	2.51	0.46
1:F:297[C]:ASP:O	1:F:298[C]:PRO:C	2.54	0.46
1:H:54[C]:LYS:NZ	1:H:192[C]:GLU:OE1	2.48	0.46
1:J:407[C]:LEU:HD23	1:J:407[C]:LEU:N	2.31	0.46
1:A:127[A]:VAL:HG23	1:A:139[A]:ILE:HD12	1.97	0.45
1:A:386[A]:PHE:CD2	1:A:461[A]:GLU:HB3	2.51	0.45
1:B:96[A]:VAL:O	1:B:100[A]:THR:HG23	2.16	0.45
1:B:289[A]:LEU:HA	1:B:289[A]:LEU:HD12	1.56	0.45
1:B:438[A]:TYR:O	2:K:155[A]:ARG:NH2	2.48	0.45
1:C:51[A]:ILE:HB	1:C:52[A]:PRO:CD	2.37	0.45
1:F:27[A]:GLN:NE2	4:F:4758[A]:HOH:O	2.46	0.45
1:F:229[A]:ILE:HG21	1:F:362[A]:PRO:CG	2.43	0.45
1:F:438[A]:TYR:HE1	2:M:133[A]:PRO:HD2	1.78	0.45
1:H:9[A]:VAL:HG22	1:H:342[A]:MET:CE	2.46	0.45
1:H:155[A]:PHE:HB2	1:H:278[A]:ILE:HD11	1.99	0.45
1:I:35[A]:ILE:CG2	1:I:117[A]:GLY:O	2.64	0.45
1:I:443[A]:GLU:OE1	2:O:134[A]:ALA:HB1	2.15	0.45
1:J:369[A]:LYS:HB2	1:J:374[A]:LEU:HD13	1.98	0.45
2:L:157[A]:ILE:HG22	2:L:158[A]:PHE:H	1.80	0.45
1:A:127[C]:VAL:HG23	1:A:139[C]:ILE:HD12	1.97	0.45
1:A:386[C]:PHE:CD2	1:A:461[C]:GLU:HB3	2.51	0.45
1:B:96[C]:VAL:O	1:B:100[C]:THR:HG23	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:289[C]:LEU:HA	1:B:289[C]:LEU:HD12	1.56	0.45
1:C:51[C]:ILE:HB	1:C:52[C]:PRO:CD	2.37	0.45
4:E:4758[C]:HOH:O	1:F:27[C]:GLN:NE2	2.46	0.45
1:F:229[C]:ILE:HG21	1:F:362[C]:PRO:CG	2.43	0.45
1:H:9[C]:VAL:HG22	1:H:342[C]:MET:CE	2.46	0.45
1:H:155[C]:PHE:HB2	1:H:278[C]:ILE:HD11	1.99	0.45
1:I:35[C]:ILE:CG2	1:I:117[C]:GLY:O	2.64	0.45
1:J:369[C]:LYS:HB2	1:J:374[C]:LEU:HD13	1.98	0.45
1:B:124[A]:LYS:HB2	1:B:124[A]:LYS:HE2	1.60	0.45
1:D:146[A]:ILE:HG23	1:D:148[A]:THR:HG23	1.99	0.45
1:E:143[A]:ASN:ND2	1:E:342[A]:MET:HE2	2.31	0.45
1:I:275[A]:LEU:HD22	1:I:276[A]:VAL:N	2.31	0.45
1:I:352[A]:ASN:ND2	1:I:369[A]:LYS:CG	2.79	0.45
2:O:156[A]:GLY:C	2:O:157[A]:ILE:HG13	2.35	0.45
1:B:124[C]:LYS:HB2	1:B:124[C]:LYS:HE2	1.60	0.45
1:D:146[C]:ILE:HG23	1:D:148[C]:THR:HG23	1.99	0.45
1:E:143[C]:ASN:ND2	1:E:342[C]:MET:HE2	2.31	0.45
1:I:275[C]:LEU:HD22	1:I:276[C]:VAL:N	2.31	0.45
1:I:352[C]:ASN:ND2	1:I:369[C]:LYS:CG	2.79	0.45
2:N:133[C]:PRO:CA	2:N:136[C]:ARG:HH21	2.28	0.45
1:A:412[A]:THR:CG2	2:K:161[A]:GLU:HG3	2.46	0.45
1:B:364[A]:VAL:HG22	1:B:421[A]:LEU:HD13	1.97	0.45
1:B:447[A]:ARG:HA	1:B:447[A]:ARG:HD2	1.55	0.45
1:C:44[A]:THR:CG2	3:C:4752[A]:FAD:PA	3.04	0.45
1:D:69[A]:LYS:HZ3	1:D:73[A]:SER:HB3	1.81	0.45
1:E:246[A]:ALA:HB1	1:E:254[A]:ILE:HD11	1.99	0.45
1:F:143[A]:ASN:HB2	1:F:342[A]:MET:HE1	1.98	0.45
1:H:351[A]:TYR:O	1:H:354[A]:VAL:HG13	2.17	0.45
1:I:9[A]:VAL:HG21	1:I:342[A]:MET:CE	2.47	0.45
1:J:144[A]:ILE:HD12	1:J:145[A]:LEU:N	2.31	0.45
2:K:130[A]:ARG:NH1	2:K:130[A]:ARG:CG	2.73	0.45
2:L:136[A]:ARG:HE	2:L:136[A]:ARG:HB2	1.35	0.45
2:M:131[A]:LEU:HD22	2:M:136[A]:ARG:HG3	1.98	0.45
1:B:364[C]:VAL:HG22	1:B:421[C]:LEU:HD13	1.97	0.45
1:B:447[C]:ARG:HA	1:B:447[C]:ARG:HD2	1.55	0.45
3:B:4752[C]:FAD:PA	1:C:44[C]:THR:CG2	3.04	0.45
1:D:69[C]:LYS:HZ3	1:D:73[C]:SER:HB3	1.81	0.45
1:E:246[C]:ALA:HB1	1:E:254[C]:ILE:HD11	1.99	0.45
1:F:143[C]:ASN:HB2	1:F:342[C]:MET:HE1	1.98	0.45
1:H:351[C]:TYR:O	1:H:354[C]:VAL:HG13	2.17	0.45
1:I:9[C]:VAL:HG21	1:I:342[C]:MET:CE	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:144[C]:ILE:HD12	1:J:145[C]:LEU:N	2.31	0.45
2:M:131[C]:LEU:HD22	2:M:136[C]:ARG:HA	1.98	0.45
1:A:254[A]:ILE:O	1:A:270[A]:THR:HA	2.16	0.45
1:A:284[A]:THR:HG22	1:A:287[A]:LEU:HD23	1.99	0.45
1:B:149[A]:GLY:HA3	3:B:4751[A]:FAD:H51A	1.97	0.45
1:C:431[A]:GLU:O	1:C:432[A]:ALA:C	2.54	0.45
1:F:137[A]:GLN:HE21	1:F:138[A]:VAL:N	2.13	0.45
1:G:436[A]:LEU:HD12	1:G:436[A]:LEU:HA	1.72	0.45
1:H:59[A]:ASN:OD1	1:H:91[A]:GLN:HG2	2.17	0.45
2:N:167[A]:VAL:O	2:N:171[A]:GLN:N	2.50	0.45
2:O:152[A]:THR:O	2:O:152[A]:THR:HG22	2.15	0.45
1:A:254[C]:ILE:O	1:A:270[C]:THR:HA	2.16	0.45
1:A:284[C]:THR:HG22	1:A:287[C]:LEU:HD23	1.99	0.45
3:A:4751[C]:FAD:H51A	1:B:149[C]:GLY:HA3	1.97	0.45
1:C:431[C]:GLU:O	1:C:432[C]:ALA:C	2.54	0.45
1:F:137[C]:GLN:HE21	1:F:138[C]:VAL:N	2.13	0.45
1:G:436[C]:LEU:HD12	1:G:436[C]:LEU:HA	1.72	0.45
1:H:59[C]:ASN:OD1	1:H:91[C]:GLN:HG2	2.17	0.45
1:C:160[A]:ILE:HA	1:C:165[A]:ILE:HG22	1.99	0.45
1:D:239[A]:LEU:O	1:D:241[A]:THR:HG23	2.16	0.45
1:E:370[A]:SER:OG	1:E:373[A]:GLN:HG3	2.17	0.45
1:I:17[A]:GLY:N	1:I:20[A]:VAL:HG13	2.32	0.45
2:K:136[A]:ARG:O	2:K:137[A]:ASN:C	2.54	0.45
1:C:160[C]:ILE:HA	1:C:165[C]:ILE:HG22	1.99	0.45
1:D:239[C]:LEU:O	1:D:241[C]:THR:HG23	2.16	0.45
1:E:370[C]:SER:OG	1:E:373[C]:GLN:HG3	2.17	0.45
1:I:17[C]:GLY:N	1:I:20[C]:VAL:HG13	2.32	0.45
1:A:155[A]:PHE:CE2	1:A:158[A]:ILE:HD12	2.51	0.45
1:A:209[A]:PHE:CE1	1:A:261[A]:ALA:HB1	2.52	0.45
1:C:87[A]:LYS:HD3	1:C:87[A]:LYS:HA	1.76	0.45
1:D:275[A]:LEU:CD2	1:D:276[A]:VAL:N	2.79	0.45
1:H:409[A]:GLN:N	1:H:416[A]:LEU:HD11	2.32	0.45
1:H:451[A]:ALA:O	1:H:454[A]:THR:OG1	2.33	0.45
1:I:225[A]:ASN:O	1:I:229[A]:ILE:HG12	2.17	0.45
2:L:142[A]:HIS:O	2:L:143[A]:SER:C	2.55	0.45
2:N:139[A]:LEU:HD11	2:N:158[A]:PHE:CZ	2.52	0.45
1:A:155[C]:PHE:CE2	1:A:158[C]:ILE:HD12	2.51	0.45
1:A:209[C]:PHE:CE1	1:A:261[C]:ALA:HB1	2.52	0.45
1:C:87[C]:LYS:HD3	1:C:87[C]:LYS:HA	1.76	0.45
1:D:275[C]:LEU:CD2	1:D:276[C]:VAL:N	2.79	0.45
1:H:409[C]:GLN:N	1:H:416[C]:LEU:HD11	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:451[C]:ALA:O	1:H:454[C]:THR:OG1	2.33	0.45
1:I:225[C]:ASN:O	1:I:229[C]:ILE:HG12	2.17	0.45
2:M:172[C]:THR:CG2	2:M:172[C]:THR:OG1	2.61	0.45
1:A:238[A]:LYS:HA	1:A:238[A]:LYS:CE	2.47	0.45
1:B:87[A]:LYS:HE3	4:B:4786[A]:HOH:O	2.15	0.45
1:B:137[A]:GLN:NE2	1:B:137[A]:GLN:HA	2.31	0.45
1:D:412[A]:THR:O	1:D:413[A]:ASP:HB3	2.17	0.45
1:I:19[A]:TYR:HB2	1:I:107[A]:PHE:CZ	2.52	0.45
1:I:320[A]:ASP:N	3:I:4759[A]:HOH:O	2.50	0.45
2:L:130[A]:ARG:N	2:L:155[A]:ARG:NH2	2.65	0.45
1:A:238[C]:LYS:HA	1:A:238[C]:LYS:CE	2.47	0.45
4:A:4786[C]:HOH:O	1:B:87[C]:LYS:HE3	2.15	0.45
1:B:137[C]:GLN:NE2	1:B:137[C]:GLN:HA	2.31	0.45
1:D:412[C]:THR:O	1:D:413[C]:ASP:HB3	2.17	0.45
4:H:4759[C]:HOH:O	1:I:320[C]:ASP:N	2.50	0.45
1:I:19[C]:TYR:HB2	1:I:107[C]:PHE:CZ	2.52	0.45
2:N:135[C]:ALA:HB1	2:N:163[C]:ALA:HB2	1.98	0.45
1:A:20[A]:VAL:CG2	1:A:336[A]:ILE:HG12	2.46	0.45
1:A:305[A]:ASN:ND2	1:A:309[A]:GLN:HB2	2.32	0.45
1:B:409[A]:GLN:HG2	1:B:412[A]:THR:OG1	2.17	0.45
1:C:290[A]:GLU:CD	1:C:290[A]:GLU:N	2.66	0.45
1:G:30[A]:PHE:O	1:G:32[A]:THR:CG2	2.65	0.45
1:I:121[A]:ILE:HD12	1:I:144[A]:ILE:HD12	1.98	0.45
1:I:342[A]:MET:HB3	1:I:342[A]:MET:HE3	1.84	0.45
1:I:376[A]:GLU:O	1:I:378[A]:GLY:N	2.49	0.45
1:I:396[A]:THR:HG22	1:J:55[A]:ALA:HB2	1.99	0.45
1:J:237[A]:PHE:O	1:J:238[A]:LYS:HD2	2.17	0.45
1:J:280[A]:ARG:NH1	1:J:280[A]:ARG:HG3	2.32	0.45
2:K:167[A]:VAL:HG12	2:K:168[A]:GLN:N	2.32	0.45
1:A:20[C]:VAL:CG2	1:A:336[C]:ILE:HG12	2.46	0.45
1:A:305[C]:ASN:ND2	1:A:309[C]:GLN:HB2	2.32	0.45
1:B:409[C]:GLN:HG2	1:B:412[C]:THR:OG1	2.17	0.45
1:C:290[C]:GLU:CD	1:C:290[C]:GLU:N	2.66	0.45
1:G:30[C]:PHE:O	1:G:32[C]:THR:CG2	2.65	0.45
1:I:121[C]:ILE:HD12	1:I:144[C]:ILE:HD12	1.98	0.45
1:I:342[C]:MET:HB3	1:I:342[C]:MET:HE3	1.84	0.45
1:I:376[C]:GLU:O	1:I:378[C]:GLY:N	2.49	0.45
1:I:396[C]:THR:HG22	1:J:55[C]:ALA:HB2	1.99	0.45
1:J:237[C]:PHE:O	1:J:238[C]:LYS:HD2	2.17	0.45
1:J:280[C]:ARG:NH1	1:J:280[C]:ARG:HG3	2.32	0.45
1:C:145[A]:LEU:HD23	1:C:316[A]:TYR:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:244[A]:THR:HB	1:C:257[A]:SER:HB3	1.99	0.45
1:D:19[A]:TYR:CD1	1:D:19[A]:TYR:C	2.90	0.45
1:D:24[A]:LYS:O	1:D:28[A]:LEU:HD22	2.16	0.45
1:D:151[A]:GLU:HG2	1:D:283[A]:PHE:HD1	1.81	0.45
1:D:180[A]:LYS:HD2	1:D:270[A]:THR:O	2.17	0.45
1:F:277[A]:CYS:HB2	4:F:4792[A]:HOH:O	2.15	0.45
1:H:260[A]:ALA:O	1:H:261[A]:ALA:C	2.55	0.45
1:I:7[A]:ALA:O	1:I:141[A]:THR:HA	2.17	0.45
2:M:159[A]:THR:CG2	2:M:161[A]:GLU:CD	2.85	0.45
2:N:130[A]:ARG:CA	2:N:157[A]:ILE:HG22	2.46	0.45
1:C:145[C]:LEU:HD23	1:C:316[C]:TYR:HB2	1.98	0.45
1:C:244[C]:THR:HB	1:C:257[C]:SER:HB3	1.99	0.45
1:D:19[C]:TYR:CD1	1:D:19[C]:TYR:C	2.90	0.45
1:D:24[C]:LYS:O	1:D:28[C]:LEU:HD22	2.16	0.45
1:D:151[C]:GLU:HG2	1:D:283[C]:PHE:HD1	1.81	0.45
1:D:180[C]:LYS:HD2	1:D:270[C]:THR:O	2.17	0.45
4:E:4792[C]:HOH:O	1:F:277[C]:CYS:HB2	2.15	0.45
1:H:260[C]:ALA:O	1:H:261[C]:ALA:C	2.55	0.45
1:I:7[C]:ALA:O	1:I:141[C]:THR:HA	2.17	0.45
1:A:92[A]:LYS:CG	1:A:93[A]:SER:N	2.76	0.45
1:C:111[A]:LYS:HB3	1:C:111[A]:LYS:HE3	1.75	0.45
1:C:451[A]:ALA:H	1:D:430[A]:ASN:ND2	2.12	0.45
1:E:438[A]:TYR:CD2	1:F:438[A]:TYR:CD2	3.05	0.45
1:E:472[A]:ILE:HD13	1:E:472[A]:ILE:C	2.36	0.45
1:F:19[A]:TYR:CD1	1:F:19[A]:TYR:C	2.90	0.45
1:F:97[A]:LYS:O	1:F:98[A]:ALA:C	2.55	0.45
1:H:46[A]:LEU:HA	1:H:51[A]:ILE:HG12	1.98	0.45
1:H:346[A]:ALA:HB1	2:N:140[A]:GLU:HG2	1.98	0.45
1:I:148[A]:THR:O	3:I:4758[A]:FAD:H8A	2.17	0.45
1:I:382[A]:LYS:HD2	1:I:466[A]:ALA:O	2.17	0.45
1:J:443[A]:GLU:HB2	1:J:467[A]:SER:OG	2.17	0.45
2:M:167[A]:VAL:HA	2:M:170[A]:LYS:CG	2.46	0.45
1:A:92[C]:LYS:CG	1:A:93[C]:SER:N	2.76	0.45
1:C:111[C]:LYS:HB3	1:C:111[C]:LYS:HE3	1.75	0.45
1:C:451[C]:ALA:H	1:D:430[C]:ASN:ND2	2.12	0.45
1:E:438[C]:TYR:CD2	1:F:438[C]:TYR:CD2	3.05	0.45
1:E:472[C]:ILE:HD13	1:E:472[C]:ILE:C	2.36	0.45
1:F:19[C]:TYR:CD1	1:F:19[C]:TYR:C	2.90	0.45
1:F:97[C]:LYS:O	1:F:98[C]:ALA:C	2.55	0.45
1:H:46[C]:LEU:HA	1:H:51[C]:ILE:HG12	1.98	0.45
3:H:4758[C]:FAD:H8A	1:I:148[C]:THR:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:382[C]:LYS:HD2	1:I:466[C]:ALA:O	2.17	0.45
1:J:443[C]:GLU:HB2	1:J:467[C]:SER:OG	2.17	0.45
1:A:430[A]:ASN:ND2	1:B:451[A]:ALA:H	2.08	0.44
1:G:49[A]:GLY:O	1:G:52[A]:PRO:HD2	2.17	0.44
1:G:178[A]:PRO:CB	1:G:273[A]:VAL:HG23	2.47	0.44
1:G:196[A]:VAL:O	1:G:200[A]:LEU:HD22	2.16	0.44
1:G:461[A]:GLU:OE1	1:G:473[A]:ASN:HB2	2.17	0.44
1:I:352[A]:ASN:ND2	1:I:369[A]:LYS:HG3	2.31	0.44
1:J:37[A]:LYS:HZ2	4:J:4759[A]:FAD:C2B	2.27	0.44
1:J:327[A]:LEU:C	4:J:4759[A]:FAD:O3'	2.56	0.44
1:A:430[C]:ASN:ND2	1:B:451[C]:ALA:H	2.08	0.44
1:G:49[C]:GLY:O	1:G:52[C]:PRO:HD2	2.17	0.44
1:G:178[C]:PRO:CB	1:G:273[C]:VAL:HG23	2.47	0.44
1:G:196[C]:VAL:O	1:G:200[C]:LEU:HD22	2.16	0.44
1:G:461[C]:GLU:OE1	1:G:473[C]:ASN:HB2	2.17	0.44
1:I:352[C]:ASN:ND2	1:I:369[C]:LYS:HG3	2.31	0.44
3:I:4759[C]:FAD:O3'	1:J:327[C]:LEU:C	2.56	0.44
3:I:4759[C]:FAD:C2B	1:J:37[C]:LYS:HZ2	2.27	0.44
1:A:380[A]:GLU:OE1	1:A:380[A]:GLU:HA	2.18	0.44
1:B:335[A]:GLY:O	1:B:339[A]:VAL:HG13	2.17	0.44
1:C:74[A]:ARG:CD	1:D:59[A]:ASN:OD1	2.45	0.44
1:C:364[A]:VAL:HG22	1:C:421[A]:LEU:HD13	1.99	0.44
1:C:382[A]:LYS:H	1:C:382[A]:LYS:HG2	1.66	0.44
1:D:278[A]:ILE:O	1:D:278[A]:ILE:CG2	2.64	0.44
1:E:249[A]:LYS:O	1:E:251[A]:ASP:O	2.34	0.44
1:E:312[A]:ILE:CG2	1:E:315[A]:ILE:HD12	2.48	0.44
1:F:46[A]:LEU:HD12	1:F:51[A]:ILE:HG13	1.98	0.44
1:G:448[A]:VAL:HG22	1:H:437[A]:GLU:HG3	1.99	0.44
1:H:242[A]:LYS:HG2	1:H:261[A]:ALA:HA	1.99	0.44
1:H:354[A]:VAL:HA	1:H:355[A]:PRO:HD3	1.72	0.44
1:I:83[A]:LEU:HD21	1:I:200[A]:LEU:HD13	1.98	0.44
1:I:383[A]:VAL:O	1:I:383[A]:VAL:CG1	2.66	0.44
1:I:442[A]:CYS:HA	1:I:463[A]:ASN:HD22	1.82	0.44
1:J:83[A]:LEU:HD22	1:J:84[A]:ASN:N	2.33	0.44
2:L:161[A]:GLU:O	2:L:165[A]:LYS:HG3	2.17	0.44
2:M:144[A]:LEU:CD2	2:M:170[A]:LYS:HE3	2.47	0.44
2:M:167[A]:VAL:HA	2:M:170[A]:LYS:HG2	2.00	0.44
1:A:380[C]:GLU:OE1	1:A:380[C]:GLU:HA	2.18	0.44
1:B:335[C]:GLY:O	1:B:339[C]:VAL:HG13	2.17	0.44
1:C:74[C]:ARG:CD	1:D:59[C]:ASN:OD1	2.45	0.44
1:C:364[C]:VAL:HG22	1:C:421[C]:LEU:HD13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:382[C]:LYS:H	1:C:382[C]:LYS:HG2	1.66	0.44
1:D:278[C]:ILE:O	1:D:278[C]:ILE:CG2	2.64	0.44
1:E:249[C]:LYS:O	1:E:251[C]:ASP:O	2.34	0.44
1:E:312[C]:ILE:CG2	1:E:315[C]:ILE:HD12	2.48	0.44
1:F:46[C]:LEU:HD12	1:F:51[C]:ILE:HG13	1.98	0.44
1:G:448[C]:VAL:HG22	1:H:437[C]:GLU:HG3	1.99	0.44
1:H:242[C]:LYS:HG2	1:H:261[C]:ALA:HA	1.99	0.44
1:H:354[C]:VAL:HA	1:H:355[C]:PRO:HD3	1.72	0.44
1:I:83[C]:LEU:HD21	1:I:200[C]:LEU:HD13	1.98	0.44
1:I:383[C]:VAL:O	1:I:383[C]:VAL:CG1	2.66	0.44
1:I:442[C]:CYS:HA	1:I:463[C]:ASN:HD22	1.82	0.44
1:J:83[C]:LEU:HD22	1:J:84[C]:ASN:N	2.33	0.44
1:A:110[A]:ASN:O	1:A:111[A]:LYS:HB3	2.17	0.44
1:C:99[A]:LEU:HA	1:C:99[A]:LEU:HD12	1.68	0.44
1:C:138[A]:VAL:C	1:C:139[A]:ILE:HG12	2.38	0.44
1:C:428[A]:MET:HE2	4:C:4801[A]:HOH:O	2.17	0.44
1:D:81[A]:VAL:O	1:D:82[A]:ARG:HD2	2.17	0.44
1:E:320[A]:ASP:OD1	1:E:326[A]:MET:HB3	2.17	0.44
1:F:193[A]:LEU:HA	1:F:193[A]:LEU:HD23	1.79	0.44
1:F:374[A]:LEU:HA	1:F:374[A]:LEU:HD12	1.66	0.44
1:I:155[A]:PHE:HD1	1:I:278[A]:ILE:HG13	1.82	0.44
1:I:468[A]:PHE:O	1:I:469[A]:GLY:C	2.56	0.44
1:J:305[A]:ASN:HD22	1:J:305[A]:ASN:N	2.11	0.44
2:M:154[A]:PRO:C	2:M:156[A]:GLY:H	2.21	0.44
1:A:110[C]:ASN:O	1:A:111[C]:LYS:HB3	2.17	0.44
4:B:4801[C]:HOH:O	1:C:428[C]:MET:HE2	2.17	0.44
1:C:99[C]:LEU:HA	1:C:99[C]:LEU:HD12	1.68	0.44
1:C:138[C]:VAL:C	1:C:139[C]:ILE:HG12	2.38	0.44
1:D:81[C]:VAL:O	1:D:82[C]:ARG:HD2	2.17	0.44
1:E:320[C]:ASP:OD1	1:E:326[C]:MET:HB3	2.17	0.44
1:F:193[C]:LEU:HD23	1:F:193[C]:LEU:HA	1.79	0.44
1:F:374[C]:LEU:HD12	1:F:374[C]:LEU:HA	1.66	0.44
1:I:155[C]:PHE:HD1	1:I:278[C]:ILE:HG13	1.82	0.44
1:I:468[C]:PHE:O	1:I:469[C]:GLY:C	2.56	0.44
1:J:305[C]:ASN:HD22	1:J:305[C]:ASN:N	2.11	0.44
1:B:189[A]:ILE:O	1:B:193[A]:LEU:HD13	2.16	0.44
1:B:346[A]:ALA:HB1	2:K:140[A]:GLU:OE2	2.17	0.44
1:C:443[A]:GLU:OE2	1:C:447[A]:ARG:NH1	2.51	0.44
1:E:395[A]:LYS:HE2	1:F:98[A]:ALA:CB	2.47	0.44
1:G:44[A]:THR:CG2	3:G:4756[A]:FAD:O2A	2.58	0.44
1:G:110[A]:ASN:O	1:G:111[A]:LYS:CG	2.58	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:124[A]:LYS:HE2	1:G:124[A]:LYS:HB3	1.73	0.44
1:G:145[A]:LEU:HD23	1:G:145[A]:LEU:HA	1.73	0.44
1:I:334[A]:GLU:O	1:I:338[A]:CYS:HB2	2.17	0.44
1:I:427[A]:GLU:OE1	1:I:427[A]:GLU:HA	2.17	0.44
1:I:464[A]:LEU:CD2	1:I:471[A]:SER:HA	2.44	0.44
1:J:242[A]:LYS:HE3	1:J:259[A]:GLU:HB3	2.00	0.44
1:J:290[A]:GLU:H	1:J:290[A]:GLU:HG3	1.57	0.44
1:J:369[A]:LYS:HB3	1:J:373[A]:GLN:HE21	1.83	0.44
2:L:167[A]:VAL:O	2:L:171[A]:GLN:HG2	2.16	0.44
1:B:189[C]:ILE:O	1:B:193[C]:LEU:HD13	2.16	0.44
1:C:443[C]:GLU:OE2	1:C:447[C]:ARG:NH1	2.51	0.44
1:E:395[C]:LYS:HE2	1:F:98[C]:ALA:CB	2.47	0.44
3:F:4756[C]:FAD:O2A	1:G:44[C]:THR:CG2	2.58	0.44
1:G:110[C]:ASN:O	1:G:111[C]:LYS:CG	2.58	0.44
1:G:124[C]:LYS:HE2	1:G:124[C]:LYS:HB3	1.73	0.44
1:G:145[C]:LEU:HD23	1:G:145[C]:LEU:HA	1.73	0.44
1:I:334[C]:GLU:O	1:I:338[C]:CYS:HB2	2.17	0.44
1:I:427[C]:GLU:OE1	1:I:427[C]:GLU:HA	2.17	0.44
1:I:464[C]:LEU:CD2	1:I:471[C]:SER:HA	2.44	0.44
1:J:242[C]:LYS:HE3	1:J:259[C]:GLU:HB3	2.00	0.44
1:J:290[C]:GLU:H	1:J:290[C]:GLU:HG3	1.57	0.44
1:J:369[C]:LYS:HB3	1:J:373[C]:GLN:HE21	1.83	0.44
2:K:159[C]:THR:HG21	2:K:161[C]:GLU:CD	2.38	0.44
1:B:219[A]:ASP:OD2	1:B:222[A]:ILE:HG23	2.17	0.44
1:C:430[A]:ASN:ND2	1:D:456[A]:SER:CB	2.58	0.44
1:E:39[A]:GLU:OE1	1:E:39[A]:GLU:HA	2.16	0.44
1:E:76[A]:ILE:O	1:E:78[A]:MET:HE1	2.17	0.44
1:H:246[A]:ALA:HA	1:H:255[A]:ASP:O	2.18	0.44
1:I:336[A]:ILE:HG22	1:I:337[A]:ILE:H	1.82	0.44
1:J:473[A]:ASN:HB3	4:J:4780[A]:HOH:O	2.18	0.44
2:M:167[A]:VAL:C	2:M:170[A]:LYS:HG3	2.38	0.44
1:B:219[C]:ASP:OD2	1:B:222[C]:ILE:HG23	2.17	0.44
1:C:430[C]:ASN:ND2	1:D:456[C]:SER:CB	2.58	0.44
1:E:39[C]:GLU:OE1	1:E:39[C]:GLU:HA	2.16	0.44
1:E:76[C]:ILE:O	1:E:78[C]:MET:HE1	2.17	0.44
1:H:246[C]:ALA:HA	1:H:255[C]:ASP:O	2.18	0.44
1:I:336[C]:ILE:HG22	1:I:337[C]:ILE:H	1.82	0.44
4:I:4781[C]:HOH:O	1:J:473[C]:ASN:HB3	2.18	0.44
2:M:150[C]:THR:CG2	2:M:151[C]:ALA:N	2.81	0.44
1:D:59[A]:ASN:HD21	1:D:91[A]:GLN:CG	2.30	0.44
1:D:146[A]:ILE:O	1:D:317[A]:ALA:HA	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:150[A]:SER:HB2	1:D:281[A]:ARG:O	2.17	0.44
1:G:177[A]:VAL:CG1	1:G:200[A]:LEU:HB3	2.36	0.44
1:H:70[A]:ASP:C	1:H:70[A]:ASP:OD1	2.56	0.44
1:I:11[A]:VAL:HB	1:I:34[A]:CYS:SG	2.58	0.44
1:I:218[A]:ILE:HD12	1:I:366[A]:TRP:CH2	2.53	0.44
1:J:46[A]:LEU:HA	1:J:51[A]:ILE:CG1	2.48	0.44
1:D:59[C]:ASN:HD21	1:D:91[C]:GLN:CG	2.30	0.44
1:D:146[C]:ILE:O	1:D:317[C]:ALA:HA	2.18	0.44
1:D:150[C]:SER:HB2	1:D:281[C]:ARG:O	2.17	0.44
1:G:177[C]:VAL:CG1	1:G:200[C]:LEU:HB3	2.36	0.44
1:H:70[C]:ASP:C	1:H:70[C]:ASP:OD1	2.56	0.44
1:I:11[C]:VAL:HB	1:I:34[C]:CYS:SG	2.58	0.44
1:I:218[C]:ILE:HD12	1:I:366[C]:TRP:CH2	2.53	0.44
1:J:46[C]:LEU:HA	1:J:51[C]:ILE:CG1	2.48	0.44
1:A:79[A]:SER:HB2	1:B:80[A]:GLU:HG2	1.98	0.44
1:B:287[A]:LEU:HD12	1:B:287[A]:LEU:HA	1.82	0.44
1:B:305[A]:ASN:ND2	1:B:309[A]:GLN:H	2.15	0.44
1:C:322[A]:VAL:HG13	1:C:323[A]:ALA:N	2.32	0.44
1:C:353[A]:CYS:HB3	1:C:437[A]:GLU:OE1	2.18	0.44
1:D:137[A]:GLN:NE2	1:D:138[A]:VAL:O	2.49	0.44
1:D:145[A]:LEU:HD11	1:D:318[A]:ILE:HG23	1.98	0.44
1:D:165[A]:ILE:HD11	1:D:254[A]:ILE:CG1	2.46	0.44
1:E:227[A]:GLN:HE21	1:E:231[A]:GLN:NE2	2.16	0.44
1:G:228[A]:ARG:NH2	1:G:229[A]:ILE:HD11	2.33	0.44
1:H:143[A]:ASN:CG	1:H:342[A]:MET:HE3	2.38	0.44
1:H:285[A]:LYS:CB	4:H:4820[A]:HOH:O	2.66	0.44
1:H:356[A]:SER:O	1:H:365[A]:ALA:HA	2.17	0.44
1:I:295[A]:GLU:O	1:I:296[A]:LEU:HG	2.18	0.44
1:J:285[A]:LYS:HD3	1:J:285[A]:LYS:HA	1.80	0.44
2:K:155[A]:ARG:NH2	2:K:157[A]:ILE:HG12	2.33	0.44
2:L:159[A]:THR:O	2:L:160[A]:LYS:C	2.56	0.44
2:L:165[A]:LYS:O	2:L:166[A]:LEU:C	2.56	0.44
2:N:168[A]:GLN:NE2	2:N:171[A]:GLN:OE1	2.45	0.44
1:A:79[C]:SER:HB2	1:B:80[C]:GLU:HG2	1.98	0.44
1:B:287[C]:LEU:HD12	1:B:287[C]:LEU:HA	1.82	0.44
1:B:305[C]:ASN:ND2	1:B:309[C]:GLN:H	2.15	0.44
1:C:322[C]:VAL:HG13	1:C:323[C]:ALA:N	2.32	0.44
1:C:353[C]:CYS:HB3	1:C:437[C]:GLU:OE1	2.18	0.44
1:D:137[C]:GLN:NE2	1:D:138[C]:VAL:O	2.49	0.44
1:D:145[C]:LEU:HD11	1:D:318[C]:ILE:HG23	1.98	0.44
1:D:165[C]:ILE:HD11	1:D:254[C]:ILE:CG1	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:227[C]:GLN:HE21	1:E:231[C]:GLN:NE2	2.16	0.44
1:G:228[C]:ARG:NH2	1:G:229[C]:ILE:HD11	2.33	0.44
4:G:4820[C]:HOH:O	1:H:285[C]:LYS:CB	2.66	0.44
1:H:143[C]:ASN:CG	1:H:342[C]:MET:HE3	2.38	0.44
1:H:356[C]:SER:O	1:H:365[C]:ALA:HA	2.17	0.44
1:I:295[C]:GLU:O	1:I:296[C]:LEU:HG	2.18	0.44
1:J:285[C]:LYS:HD3	1:J:285[C]:LYS:HA	1.80	0.44
1:B:164[A]:THR:HG21	1:B:248[A]:LYS:HZ1	1.83	0.44
1:B:369[A]:LYS:HB2	1:B:374[A]:LEU:HD13	2.00	0.44
1:C:318[A]:ILE:HD12	1:C:335[A]:GLY:HA2	2.00	0.44
1:E:297[A]:ASP:C	1:E:297[A]:ASP:OD1	2.56	0.44
1:J:57[A]:LEU:O	1:J:199[A]:ARG:NH1	2.51	0.44
1:J:246[A]:ALA:C	1:J:247[A]:THR:HG22	2.37	0.44
1:J:249[A]:LYS:HD3	1:J:255[A]:ASP:CG	2.38	0.44
1:J:259[A]:GLU:CG	1:J:264[A]:GLY:HA2	2.44	0.44
2:L:139[A]:LEU:HD23	2:L:144[A]:LEU:HD13	1.99	0.44
2:M:152[A]:THR:HB	2:M:162[A]:ASP:OD1	2.17	0.44
2:N:133[A]:PRO:HB3	2:N:136[A]:ARG:HH21	1.82	0.44
1:B:164[C]:THR:HG21	1:B:248[C]:LYS:HZ1	1.83	0.44
1:B:369[C]:LYS:HB2	1:B:374[C]:LEU:HD13	2.00	0.44
1:C:318[C]:ILE:HD12	1:C:335[C]:GLY:HA2	2.00	0.44
1:E:297[C]:ASP:C	1:E:297[C]:ASP:OD1	2.56	0.44
1:E:444[C]:ASP:OD1	2:M:155[C]:ARG:HD3	2.18	0.44
1:J:57[C]:LEU:O	1:J:199[C]:ARG:NH1	2.51	0.44
1:J:246[C]:ALA:C	1:J:247[C]:THR:HG22	2.37	0.44
1:J:249[C]:LYS:HD3	1:J:255[C]:ASP:CG	2.38	0.44
1:J:259[C]:GLU:CG	1:J:264[C]:GLY:HA2	2.44	0.44
2:K:150[C]:THR:HG22	2:K:151[C]:ALA:N	2.32	0.44
1:B:5[A]:ILE:HG21	1:B:5[A]:ILE:HD13	1.57	0.44
1:C:409[A]:GLN:NE2	1:C:411[A]:SER:H	2.16	0.44
1:D:143[A]:ASN:ND2	1:D:342[A]:MET:CE	2.81	0.44
1:E:241[A]:THR:HG22	1:E:242[A]:LYS:N	2.33	0.44
1:F:213[A]:VAL:HG22	4:F:4763[A]:HOH:O	2.17	0.44
1:G:314[A]:ASN:ND2	1:G:314[A]:ASN:N	2.59	0.44
1:G:354[A]:VAL:HA	1:G:355[A]:PRO:HD3	1.77	0.44
1:H:275[A]:LEU:HD12	1:H:276[A]:VAL:H	1.83	0.44
1:J:144[A]:ILE:HG23	1:J:315[A]:ILE:HG12	2.00	0.44
1:J:414[A]:ARG:HA	1:J:441[A]:SER:HA	1.99	0.44
2:K:144[A]:LEU:C	2:K:144[A]:LEU:HD12	2.38	0.44
2:M:139[A]:LEU:O	2:M:143[A]:SER:N	2.51	0.44
1:B:5[C]:ILE:HG21	1:B:5[C]:ILE:HD13	1.57	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:409[C]:GLN:NE2	1:C:411[C]:SER:H	2.16	0.44
1:D:143[C]:ASN:ND2	1:D:342[C]:MET:CE	2.81	0.44
1:E:241[C]:THR:HG22	1:E:242[C]:LYS:N	2.33	0.44
4:E:4763[C]:HOH:O	1:F:213[C]:VAL:HG22	2.17	0.44
1:G:314[C]:ASN:ND2	1:G:314[C]:ASN:N	2.59	0.44
1:G:354[C]:VAL:HA	1:G:355[C]:PRO:HD3	1.77	0.44
1:H:275[C]:LEU:HD12	1:H:276[C]:VAL:H	1.83	0.44
1:J:144[C]:ILE:HG23	1:J:315[C]:ILE:HG12	2.00	0.44
1:J:414[C]:ARG:HA	1:J:441[C]:SER:HA	1.99	0.44
2:L:138[C]:ILE:CG1	2:L:167[C]:VAL:HG21	2.48	0.44
1:A:45[A]:CYS:O	1:A:50[A]:CYS:HB2	2.17	0.43
1:B:145[A]:LEU:HD11	1:B:318[A]:ILE:HG23	1.98	0.43
1:D:172[A]:LEU:HD12	1:D:172[A]:LEU:HA	1.79	0.43
1:D:339[A]:VAL:HA	1:D:342[A]:MET:HG3	2.00	0.43
1:D:450[A]:HIS:CD2	1:D:460[A]:ARG:HB2	2.53	0.43
1:I:320[A]:ASP:HB3	1:I:326[A]:MET:HE3	2.00	0.43
1:I:471[A]:SER:OG	1:I:474[A]:PHE:O	2.26	0.43
1:J:33[A]:VAL:CG1	1:J:34[A]:CYS:N	2.79	0.43
2:K:159[A]:THR:N	2:K:162[A]:ASP:HB2	2.32	0.43
1:A:45[C]:CYS:O	1:A:50[C]:CYS:HB2	2.17	0.43
1:B:145[C]:LEU:HD11	1:B:318[C]:ILE:HG23	1.98	0.43
1:D:172[C]:LEU:HD12	1:D:172[C]:LEU:HA	1.79	0.43
1:D:339[C]:VAL:HA	1:D:342[C]:MET:HG3	2.00	0.43
1:D:450[C]:HIS:CD2	1:D:460[C]:ARG:HB2	2.53	0.43
1:I:320[C]:ASP:HB3	1:I:326[C]:MET:HE3	2.00	0.43
1:I:471[C]:SER:OG	1:I:474[C]:PHE:O	2.26	0.43
1:J:33[C]:VAL:CG1	1:J:34[C]:CYS:N	2.79	0.43
1:A:184[A]:ILE:HD11	1:A:274[A]:LEU:HD11	2.00	0.43
1:A:188[A]:VAL:HG23	1:A:189[A]:ILE:CD1	2.41	0.43
1:B:11[A]:VAL:HG22	1:B:145[A]:LEU:HD23	1.99	0.43
1:B:19[A]:TYR:HB2	1:B:107[A]:PHE:CZ	2.52	0.43
1:B:333[A]:ASP:O	1:B:337[A]:ILE:HG23	2.17	0.43
1:C:404[A]:VAL:HG11	1:C:459[A]:PHE:HA	2.00	0.43
1:D:409[A]:GLN:HE21	1:D:411[A]:SER:N	1.92	0.43
1:G:61[A]:HIS:HB2	1:G:199[A]:ARG:NH1	2.34	0.43
1:G:380[A]:GLU:HA	1:G:380[A]:GLU:OE1	2.18	0.43
1:G:395[A]:LYS:HD2	1:G:395[A]:LYS:HA	1.83	0.43
1:I:453[A]:PRO:C	1:I:454[A]:THR:CG2	2.87	0.43
1:J:463[A]:ASN:HD22	1:J:463[A]:ASN:HA	1.53	0.43
2:N:150[A]:THR:O	2:N:162[A]:ASP:OD1	2.37	0.43
1:A:184[C]:ILE:HD11	1:A:274[C]:LEU:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188[C]:VAL:HG23	1:A:189[C]:ILE:CD1	2.41	0.43
1:B:11[C]:VAL:HG22	1:B:145[C]:LEU:HD23	1.99	0.43
1:B:19[C]:TYR:HB2	1:B:107[C]:PHE:CZ	2.52	0.43
1:B:333[C]:ASP:O	1:B:337[C]:ILE:HG23	2.17	0.43
1:C:404[C]:VAL:HG11	1:C:459[C]:PHE:HA	2.00	0.43
1:D:409[C]:GLN:HE21	1:D:411[C]:SER:N	1.92	0.43
1:G:61[C]:HIS:HB2	1:G:199[C]:ARG:NH1	2.34	0.43
1:G:380[C]:GLU:HA	1:G:380[C]:GLU:OE1	2.18	0.43
1:G:395[C]:LYS:HD2	1:G:395[C]:LYS:HA	1.83	0.43
1:I:453[C]:PRO:C	1:I:454[C]:THR:CG2	2.87	0.43
1:J:463[C]:ASN:HD22	1:J:463[C]:ASN:HA	1.53	0.43
2:M:131[C]:LEU:HB3	2:M:136[C]:ARG:HB2	2.00	0.43
2:N:158[C]:PHE:CE2	2:N:163[C]:ALA:CA	2.99	0.43
1:A:438[A]:TYR:O	2:K:154[A]:PRO:HG2	2.19	0.43
1:B:54[A]:LYS:HD2	1:B:359[A]:TYR:CG	2.53	0.43
1:C:410[A]:LYS:HE3	1:C:410[A]:LYS:HB2	1.79	0.43
1:D:329[A]:HIS:CD2	1:D:355[A]:PRO:HD2	2.53	0.43
1:E:182[A]:VAL:HG22	1:E:274[A]:LEU:HD13	1.99	0.43
1:E:369[A]:LYS:NZ	4:E:4792[A]:HOH:O	2.50	0.43
1:F:218[A]:ILE:HD12	1:F:223[A]:SER:HB2	2.00	0.43
1:G:302[A]:ILE:HA	1:G:303[A]:PRO:HD2	1.87	0.43
1:G:441[A]:SER:OG	2:N:160[A]:LYS:HD3	2.18	0.43
1:I:284[A]:THR:HG21	1:I:289[A]:LEU:HD21	1.99	0.43
1:I:427[A]:GLU:OE1	1:J:454[A]:THR:HB	2.18	0.43
2:M:152[A]:THR:HG22	2:M:153[A]:GLY:H	1.81	0.43
1:B:54[C]:LYS:HD2	1:B:359[C]:TYR:CG	2.53	0.43
1:C:410[C]:LYS:HE3	1:C:410[C]:LYS:HB2	1.79	0.43
1:D:329[C]:HIS:CD2	1:D:355[C]:PRO:HD2	2.53	0.43
4:D:4792[C]:HOH:O	1:E:369[C]:LYS:NZ	2.50	0.43
1:E:182[C]:VAL:HG22	1:E:274[C]:LEU:HD13	1.99	0.43
1:F:218[C]:ILE:HD12	1:F:223[C]:SER:HB2	2.00	0.43
1:G:302[C]:ILE:HA	1:G:303[C]:PRO:HD2	1.87	0.43
1:H:438[C]:TYR:CE1	2:N:155[C]:ARG:HD3	2.44	0.43
1:I:284[C]:THR:HG21	1:I:289[C]:LEU:HD21	1.99	0.43
1:I:427[C]:GLU:OE1	1:J:454[C]:THR:HB	2.18	0.43
2:L:132[C]:SER:HB3	2:L:135[C]:ALA:HB2	1.98	0.43
1:B:174[A]:LEU:HD12	1:B:174[A]:LEU:HA	1.77	0.43
1:B:393[A]:ARG:HA	1:B:396[A]:THR:CG2	2.47	0.43
1:C:15[A]:GLY:N	3:C:4753[A]:HOH:O	2.51	0.43
1:C:302[A]:ILE:O	1:C:304[A]:VAL:HG13	2.18	0.43
1:E:66[A]:ALA:HB2	1:F:71[A]:PHE:HE2	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:305[A]:ASN:OD1	1:F:307[A]:ARG:N	2.50	0.43
1:H:51[A]:ILE:HG23	1:H:51[A]:ILE:HD12	1.76	0.43
1:H:174[A]:LEU:HB2	1:H:197[A]:TRP:CZ2	2.53	0.43
1:I:13[A]:GLY:O	1:I:18[A]:GLY:HA3	2.18	0.43
1:I:43[A]:GLY:HA2	4:I:4761[A]:HOH:O	2.18	0.43
1:J:62[A]:TYR:HD1	1:J:65[A]:MET:CE	2.31	0.43
1:B:174[C]:LEU:HD12	1:B:174[C]:LEU:HA	1.77	0.43
1:B:393[C]:ARG:HA	1:B:396[C]:THR:CG2	2.47	0.43
4:B:4753[C]:HOH:O	1:C:15[C]:GLY:N	2.51	0.43
1:C:302[C]:ILE:O	1:C:304[C]:VAL:HG13	2.18	0.43
1:E:66[C]:ALA:HB2	1:F:71[C]:PHE:HE2	1.84	0.43
1:F:305[C]:ASN:OD1	1:F:307[C]:ARG:N	2.50	0.43
1:H:51[C]:ILE:HG23	1:H:51[C]:ILE:HD12	1.76	0.43
1:H:174[C]:LEU:HB2	1:H:197[C]:TRP:CZ2	2.53	0.43
4:H:4761[C]:HOH:O	1:I:43[C]:GLY:HA2	2.18	0.43
1:I:13[C]:GLY:O	1:I:18[C]:GLY:HA3	2.18	0.43
1:J:62[C]:TYR:HD1	1:J:65[C]:MET:CE	2.31	0.43
2:K:150[C]:THR:CG2	2:K:151[C]:ALA:N	2.82	0.43
1:B:60[A]:SER:HB2	1:B:200[A]:LEU:HD11	1.99	0.43
1:D:182[A]:VAL:HG23	1:D:271[A]:CYS:HB3	2.00	0.43
1:D:359[A]:TYR:C	1:D:360[A]:THR:O	2.53	0.43
1:F:122[A]:THR:OG1	1:F:126[A]:GLN:HG2	2.19	0.43
1:F:188[A]:VAL:HG12	1:F:189[A]:ILE:N	2.33	0.43
1:G:10[A]:THR:OG1	1:G:141[A]:THR:CG2	2.67	0.43
1:G:339[A]:VAL:C	1:G:341[A]:GLY:H	2.20	0.43
1:H:116[A]:ASN:HB3	1:H:131[A]:LYS:NZ	2.33	0.43
1:H:380[A]:GLU:HG2	1:H:410[A]:LYS:HB3	2.00	0.43
1:J:62[A]:TYR:HA	1:J:65[A]:MET:HE2	1.99	0.43
1:J:69[A]:LYS:NZ	1:J:69[A]:LYS:CB	2.81	0.43
1:J:232[A]:LYS:HE3	1:J:232[A]:LYS:CA	2.48	0.43
1:B:60[C]:SER:HB2	1:B:200[C]:LEU:HD11	1.99	0.43
1:D:182[C]:VAL:HG23	1:D:271[C]:CYS:HB3	2.00	0.43
1:D:359[C]:TYR:C	1:D:360[C]:THR:O	2.53	0.43
1:F:122[C]:THR:OG1	1:F:126[C]:GLN:HG2	2.19	0.43
1:F:188[C]:VAL:HG12	1:F:189[C]:ILE:N	2.33	0.43
1:G:10[C]:THR:OG1	1:G:141[C]:THR:CG2	2.67	0.43
1:G:339[C]:VAL:C	1:G:341[C]:GLY:H	2.20	0.43
1:H:116[C]:ASN:HB3	1:H:131[C]:LYS:NZ	2.33	0.43
1:H:380[C]:GLU:HG2	1:H:410[C]:LYS:HB3	2.00	0.43
1:J:62[C]:TYR:HA	1:J:65[C]:MET:HE2	1.99	0.43
1:J:69[C]:LYS:NZ	1:J:69[C]:LYS:CB	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:232[C]:LYS:HE3	1:J:232[C]:LYS:CA	2.48	0.43
2:M:132[C]:SER:O	2:M:134[C]:ALA:N	2.52	0.43
1:C:40[A]:THR:HG23	1:C:47[A]:ASN:ND2	2.33	0.43
1:C:407[A]:LEU:HD23	1:C:407[A]:LEU:HA	1.80	0.43
1:D:441[A]:SER:O	1:D:442[A]:CYS:C	2.56	0.43
1:E:311[A]:LYS:HB2	1:E:311[A]:LYS:HE3	1.69	0.43
1:E:464[A]:LEU:HD23	1:E:464[A]:LEU:C	2.39	0.43
1:F:354[A]:VAL:HA	1:F:355[A]:PRO:HD3	1.75	0.43
1:H:90[A]:GLU:O	1:H:91[A]:GLN:C	2.56	0.43
1:I:182[A]:VAL:HG11	1:I:269[A]:ILE:HG21	1.99	0.43
1:J:15[A]:GLY:O	1:J:19[A]:TYR:CD2	2.71	0.43
1:J:109[A]:GLN:O	1:J:111[A]:LYS:N	2.51	0.43
1:C:40[C]:THR:HG23	1:C:47[C]:ASN:ND2	2.33	0.43
1:C:407[C]:LEU:HD23	1:C:407[C]:LEU:HA	1.80	0.43
1:D:441[C]:SER:O	1:D:442[C]:CYS:C	2.56	0.43
1:E:311[C]:LYS:HB2	1:E:311[C]:LYS:HE3	1.69	0.43
1:E:464[C]:LEU:HD23	1:E:464[C]:LEU:C	2.39	0.43
1:F:354[C]:VAL:HA	1:F:355[C]:PRO:HD3	1.75	0.43
1:H:90[C]:GLU:O	1:H:91[C]:GLN:C	2.56	0.43
1:I:182[C]:VAL:HG11	1:I:269[C]:ILE:HG21	1.99	0.43
1:J:15[C]:GLY:O	1:J:19[C]:TYR:CD2	2.71	0.43
1:J:109[C]:GLN:O	1:J:111[C]:LYS:N	2.51	0.43
2:M:166[C]:LEU:O	2:M:170[C]:LYS:HB2	2.19	0.43
1:A:174[A]:LEU:HA	1:A:174[A]:LEU:HD13	1.48	0.43
1:A:387[A]:PRO:HA	1:A:403[A]:MET:HA	1.99	0.43
1:B:16[A]:PRO:O	3:B:4751[A]:FAD:O1P	2.36	0.43
1:C:381[A]:TYR:CD1	1:C:381[A]:TYR:N	2.86	0.43
1:E:330[A]:LYS:NZ	4:E:4766[A]:HOH:O	2.47	0.43
1:E:386[A]:PHE:CZ	1:E:473[A]:ASN:HB2	2.53	0.43
1:F:83[A]:LEU:HD13	1:F:85[A]:LEU:N	2.34	0.43
1:F:116[A]:ASN:C	1:F:116[A]:ASN:ND2	2.70	0.43
1:F:153[A]:THR:OG1	1:F:281[A]:ARG:HG2	2.18	0.43
1:F:168[A]:SER:O	1:F:172[A]:LEU:HD22	2.19	0.43
1:F:189[A]:ILE:HG23	3:F:4755[A]:FAD:HM73	2.01	0.43
1:G:299[A]:ARG:N	1:G:299[A]:ARG:CD	2.81	0.43
1:G:437[A]:GLU:O	2:N:154[A]:PRO:HG3	2.18	0.43
1:I:47[A]:ASN:C	1:I:48[A]:VAL:HG13	2.39	0.43
1:J:57[A]:LEU:HD11	1:J:192[A]:GLU:HG2	2.00	0.43
2:K:142[A]:HIS:O	2:K:144[A]:LEU:HG	2.19	0.43
1:A:174[C]:LEU:HA	1:A:174[C]:LEU:HD13	1.48	0.43
1:A:387[C]:PRO:HA	1:A:403[C]:MET:HA	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:4751[C]:FAD:O1P	1:B:16[C]:PRO:O	2.36	0.43
1:C:381[C]:TYR:CD1	1:C:381[C]:TYR:N	2.86	0.43
4:D:4766[C]:HOH:O	1:E:330[C]:LYS:NZ	2.47	0.43
1:E:386[C]:PHE:CZ	1:E:473[C]:ASN:HB2	2.53	0.43
3:E:4755[C]:FAD:HM73	1:F:189[C]:ILE:HG23	2.01	0.43
1:F:83[C]:LEU:HD13	1:F:85[C]:LEU:N	2.34	0.43
1:F:116[C]:ASN:C	1:F:116[C]:ASN:ND2	2.70	0.43
1:F:153[C]:THR:OG1	1:F:281[C]:ARG:HG2	2.18	0.43
1:F:168[C]:SER:O	1:F:172[C]:LEU:HD22	2.19	0.43
1:G:299[C]:ARG:N	1:G:299[C]:ARG:CD	2.81	0.43
1:I:47[C]:ASN:C	1:I:48[C]:VAL:HG13	2.39	0.43
1:J:57[C]:LEU:HD11	1:J:192[C]:GLU:HG2	2.00	0.43
1:A:155[A]:PHE:CD2	1:A:158[A]:ILE:HD12	2.54	0.43
1:D:229[A]:ILE:HD13	1:D:362[A]:PRO:HG3	1.99	0.43
1:E:155[A]:PHE:CD1	1:E:155[A]:PHE:C	2.92	0.43
1:E:453[A]:PRO:HD2	1:F:359[A]:TYR:CZ	2.54	0.43
1:G:138[A]:VAL:C	1:G:139[A]:ILE:HD12	2.39	0.43
1:H:143[A]:ASN:CG	1:H:342[A]:MET:CE	2.87	0.43
1:I:208[A]:GLU:OE1	1:I:209[A]:PHE:N	2.51	0.43
1:J:356[A]:SER:O	1:J:365[A]:ALA:HA	2.19	0.43
1:J:393[A]:ARG:HB3	1:J:455[A]:LEU:CD1	2.48	0.43
1:A:155[C]:PHE:CD2	1:A:158[C]:ILE:HD12	2.54	0.43
1:D:229[C]:ILE:HD13	1:D:362[C]:PRO:HG3	1.99	0.43
1:E:155[C]:PHE:C	1:E:155[C]:PHE:CD1	2.92	0.43
1:E:453[C]:PRO:HD2	1:F:359[C]:TYR:CZ	2.54	0.43
1:G:138[C]:VAL:C	1:G:139[C]:ILE:HD12	2.39	0.43
1:H:143[C]:ASN:CG	1:H:342[C]:MET:CE	2.87	0.43
1:I:208[C]:GLU:OE1	1:I:209[C]:PHE:N	2.51	0.43
1:J:356[C]:SER:O	1:J:365[C]:ALA:HA	2.19	0.43
1:J:393[C]:ARG:HB3	1:J:455[C]:LEU:CD1	2.48	0.43
2:K:136[C]:ARG:O	2:K:136[C]:ARG:CG	2.52	0.43
1:B:35[A]:ILE:HA	1:B:115[A]:VAL:O	2.19	0.43
1:E:3[A]:GLN:HA	1:E:4[A]:PRO:HD2	1.89	0.43
1:E:397[A]:ASN:O	1:E:398[A]:ALA:HB3	2.19	0.43
1:E:434[A]:LEU:HD12	1:F:448[A]:VAL:HG21	2.01	0.43
1:E:448[A]:VAL:HG21	1:F:434[A]:LEU:HD12	2.01	0.43
1:F:259[A]:GLU:CG	1:F:264[A]:GLY:HA2	2.48	0.43
1:I:374[A]:LEU:HD12	1:I:407[A]:LEU:HD13	2.01	0.43
1:J:362[A]:PRO:HB2	1:J:422[A]:GLY:HA2	2.00	0.43
2:L:146[A]:ALA:O	2:L:147[A]:SER:C	2.56	0.43
2:N:152[A]:THR:HG22	2:N:153[A]:GLY:H	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:35[C]:ILE:HA	1:B:115[C]:VAL:O	2.19	0.43
1:E:3[C]:GLN:HA	1:E:4[C]:PRO:HD2	1.89	0.43
1:E:397[C]:ASN:O	1:E:398[C]:ALA:HB3	2.19	0.43
1:E:434[C]:LEU:HD12	1:F:448[C]:VAL:HG21	2.01	0.43
1:E:448[C]:VAL:HG21	1:F:434[C]:LEU:HD12	2.01	0.43
1:F:259[C]:GLU:CG	1:F:264[C]:GLY:HA2	2.48	0.43
3:H:4758[C]:FAD:O2'	3:H:4758[C]:FAD:O4'	2.16	0.43
1:I:374[C]:LEU:HD12	1:I:407[C]:LEU:HD13	2.01	0.43
1:J:362[C]:PRO:HB2	1:J:422[C]:GLY:HA2	2.00	0.43
1:B:49[A]:GLY:HA2	3:B:4751[A]:FAD:HM82	2.01	0.43
1:D:155[A]:PHE:HA	1:D:156[A]:PRO:HD3	1.91	0.43
1:D:396[A]:THR:C	1:D:398[A]:ALA:H	2.22	0.43
1:D:406[A]:ILE:CD1	1:D:463[A]:ASN:CG	2.87	0.43
1:E:11[A]:VAL:HG11	1:E:18[A]:GLY:HA2	2.01	0.43
1:F:54[A]:LYS:HD3	1:F:54[A]:LYS:HA	1.84	0.43
1:F:164[A]:THR:CG2	1:F:248[A]:LYS:HE3	2.49	0.43
1:F:370[A]:SER:H	1:F:373[A]:GLN:NE2	2.17	0.43
1:F:389[A]:ALA:HA	1:F:400[A]:THR:HB	2.01	0.43
1:G:155[A]:PHE:CD2	1:G:158[A]:ILE:HG13	2.54	0.43
1:J:37[A]:LYS:HE3	4:J:4759[A]:FAD:N9A	2.33	0.43
2:L:167[A]:VAL:HG12	2:L:168[A]:GLN:N	2.34	0.43
3:A:4751[C]:FAD:HM82	1:B:49[C]:GLY:HA2	2.01	0.43
1:D:155[C]:PHE:HA	1:D:156[C]:PRO:HD3	1.91	0.43
1:D:396[C]:THR:C	1:D:398[C]:ALA:H	2.22	0.43
1:D:406[C]:ILE:CD1	1:D:463[C]:ASN:CG	2.87	0.43
1:E:11[C]:VAL:HG11	1:E:18[C]:GLY:HA2	2.01	0.43
1:F:54[C]:LYS:HD3	1:F:54[C]:LYS:HA	1.84	0.43
1:F:164[C]:THR:CG2	1:F:248[C]:LYS:HE3	2.49	0.43
1:F:370[C]:SER:H	1:F:373[C]:GLN:NE2	2.17	0.43
1:F:389[C]:ALA:HA	1:F:400[C]:THR:HB	2.01	0.43
1:G:155[C]:PHE:CD2	1:G:158[C]:ILE:HG13	2.54	0.43
3:I:4759[C]:FAD:N9A	1:J:37[C]:LYS:HE3	2.33	0.43
2:L:145[C]:ASP:O	2:L:148[C]:GLN:HG2	2.19	0.43
2:L:164[C]:LEU:O	2:L:165[C]:LYS:C	2.57	0.43
1:B:371[A]:GLU:OE1	1:B:381[A]:TYR:OH	2.27	0.42
1:D:145[A]:LEU:HD21	1:D:318[A]:ILE:CD1	2.48	0.42
1:E:354[A]:VAL:HA	1:E:355[A]:PRO:HD3	1.81	0.42
1:F:92[A]:LYS:NZ	1:F:172[A]:LEU:O	2.51	0.42
1:F:305[A]:ASN:OD1	1:F:305[A]:ASN:C	2.57	0.42
1:F:392[A]:SER:CB	4:F:4793[A]:HOH:O	2.50	0.42
1:H:5[A]:ILE:HG23	1:H:137[A]:GLN:HE22	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:44[A]:THR:HG23	3:H:4757[A]:FAD:PA	2.59	0.42
1:I:43[A]:GLY:HA2	3:I:4758[A]:FAD:O3B	2.19	0.42
1:I:453[A]:PRO:O	1:I:454[A]:THR:HG22	2.20	0.42
2:M:159[A]:THR:HB	2:M:162[A]:ASP:OD2	2.18	0.42
1:B:371[C]:GLU:OE1	1:B:381[C]:TYR:OH	2.27	0.42
1:D:145[C]:LEU:HD21	1:D:318[C]:ILE:CD1	2.48	0.42
1:E:354[C]:VAL:HA	1:E:355[C]:PRO:HD3	1.81	0.42
4:E:4793[C]:HOH:O	1:F:392[C]:SER:CB	2.50	0.42
1:F:92[C]:LYS:NZ	1:F:172[C]:LEU:O	2.51	0.42
1:F:305[C]:ASN:OD1	1:F:305[C]:ASN:C	2.57	0.42
3:G:4757[C]:FAD:PA	1:H:44[C]:THR:HG23	2.59	0.42
1:H:5[C]:ILE:HG23	1:H:137[C]:GLN:HE22	1.83	0.42
3:H:4758[C]:FAD:O3B	1:I:43[C]:GLY:HA2	2.19	0.42
1:I:453[C]:PRO:O	1:I:454[C]:THR:HG22	2.20	0.42
1:A:16[A]:PRO:HG2	1:A:45[A]:CYS:HB2	2.01	0.42
1:A:20[A]:VAL:HG23	1:A:336[A]:ILE:HG12	2.01	0.42
1:A:41[A]:LEU:HD21	1:A:114[A]:HIS:CE1	2.54	0.42
1:B:8[A]:ASP:HA	1:B:142[A]:LYS:HB2	2.01	0.42
1:D:302[A]:ILE:HD12	1:D:321[A]:VAL:HG22	2.01	0.42
1:E:278[A]:ILE:HD12	1:E:278[A]:ILE:HA	1.26	0.42
1:E:409[A]:GLN:HE21	1:E:412[A]:THR:H	1.66	0.42
1:G:196[A]:VAL:HG12	1:G:197[A]:TRP:N	2.33	0.42
1:G:381[A]:TYR:CD1	1:G:381[A]:TYR:C	2.92	0.42
1:G:426[A]:GLY:O	1:G:429[A]:VAL:HG12	2.18	0.42
1:H:358[A]:ILE:HD13	1:H:358[A]:ILE:HG21	1.82	0.42
1:I:40[A]:THR:HG21	1:I:100[A]:THR:HG21	2.00	0.42
1:I:244[A]:THR:HB	1:I:257[A]:SER:HB2	2.01	0.42
1:J:144[A]:ILE:O	1:J:144[A]:ILE:HG13	2.18	0.42
1:J:321[A]:VAL:O	1:J:321[A]:VAL:HG13	2.16	0.42
1:A:16[C]:PRO:HG2	1:A:45[C]:CYS:HB2	2.01	0.42
1:A:20[C]:VAL:HG23	1:A:336[C]:ILE:HG12	2.01	0.42
1:A:41[C]:LEU:HD21	1:A:114[C]:HIS:CE1	2.54	0.42
1:B:8[C]:ASP:HA	1:B:142[C]:LYS:HB2	2.01	0.42
1:D:302[C]:ILE:HD12	1:D:321[C]:VAL:HG22	2.01	0.42
1:E:278[C]:ILE:HD12	1:E:278[C]:ILE:HA	1.26	0.42
1:E:409[C]:GLN:HE21	1:E:412[C]:THR:H	1.66	0.42
1:G:196[C]:VAL:HG12	1:G:197[C]:TRP:N	2.33	0.42
1:G:381[C]:TYR:CD1	1:G:381[C]:TYR:C	2.92	0.42
1:G:426[C]:GLY:O	1:G:429[C]:VAL:HG12	2.18	0.42
1:H:358[C]:ILE:HD13	1:H:358[C]:ILE:HG21	1.82	0.42
1:I:40[C]:THR:HG21	1:I:100[C]:THR:HG21	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:244[C]:THR:HB	1:I:257[C]:SER:HB2	2.01	0.42
1:J:144[C]:ILE:O	1:J:144[C]:ILE:HG13	2.18	0.42
1:J:321[C]:VAL:O	1:J:321[C]:VAL:HG13	2.16	0.42
2:K:159[C]:THR:CG2	2:K:161[C]:GLU:CD	2.87	0.42
2:M:159[C]:THR:CG2	2:M:162[C]:ASP:OD1	2.66	0.42
1:A:37[A]:LYS:NZ	4:A:4767[A]:HOH:O	2.50	0.42
1:C:121[A]:ILE:CG2	1:C:292[A]:LEU:HD11	2.48	0.42
1:C:175[A]:LYS:HB2	1:C:175[A]:LYS:HE3	1.75	0.42
1:D:183[A]:VAL:HG13	1:D:275[A]:LEU:CD1	2.48	0.42
1:D:249[A]:LYS:HA	1:D:249[A]:LYS:HD2	1.73	0.42
1:E:19[A]:TYR:CD1	1:E:19[A]:TYR:C	2.92	0.42
1:G:230[A]:LEU:HD12	1:G:230[A]:LEU:HA	1.87	0.42
1:H:174[A]:LEU:HD12	1:H:174[A]:LEU:HA	1.75	0.42
1:I:94[A]:THR:O	1:I:95[A]:ALA:C	2.57	0.42
1:J:54[A]:LYS:HD2	1:J:359[A]:TYR:CG	2.53	0.42
1:J:372[A]:GLU:CD	1:J:372[A]:GLU:N	2.73	0.42
1:A:37[C]:LYS:NZ	4:J:4767[C]:HOH:O	2.50	0.42
1:C:121[C]:ILE:CG2	1:C:292[C]:LEU:HD11	2.48	0.42
1:C:175[C]:LYS:HB2	1:C:175[C]:LYS:HE3	1.75	0.42
1:D:183[C]:VAL:HG13	1:D:275[C]:LEU:CD1	2.48	0.42
1:D:249[C]:LYS:HA	1:D:249[C]:LYS:HD2	1.73	0.42
1:E:19[C]:TYR:CD1	1:E:19[C]:TYR:C	2.92	0.42
1:G:230[C]:LEU:HD12	1:G:230[C]:LEU:HA	1.87	0.42
1:H:174[C]:LEU:HD12	1:H:174[C]:LEU:HA	1.75	0.42
1:I:94[C]:THR:O	1:I:95[C]:ALA:C	2.57	0.42
1:J:54[C]:LYS:HD2	1:J:359[C]:TYR:CG	2.53	0.42
1:J:372[C]:GLU:CD	1:J:372[C]:GLU:N	2.73	0.42
2:L:145[C]:ASP:OD1	2:L:145[C]:ASP:N	2.51	0.42
2:N:130[C]:ARG:O	2:N:157[C]:ILE:HA	2.18	0.42
1:A:221[A]:GLU:HB3	1:A:405[A]:LYS:HZ1	1.84	0.42
1:B:37[A]:LYS:HG2	3:B:4751[A]:FAD:N3A	2.33	0.42
1:C:402[A]:GLY:HA3	1:C:421[A]:LEU:O	2.19	0.42
1:D:282[A]:PRO:HB3	1:D:321[A]:VAL:HA	2.01	0.42
1:E:281[A]:ARG:H	1:E:281[A]:ARG:HG2	1.52	0.42
1:I:46[A]:LEU:HD21	1:I:100[A]:THR:HG22	2.01	0.42
1:I:208[A]:GLU:OE1	1:I:208[A]:GLU:CA	2.67	0.42
1:I:241[A]:THR:HG22	1:I:260[A]:ALA:CA	2.46	0.42
1:J:388[A]:PHE:C	1:J:390[A]:ALA:N	2.72	0.42
2:M:158[A]:PHE:HE2	2:M:163[A]:ALA:HA	1.84	0.42
1:A:221[C]:GLU:HB3	1:A:405[C]:LYS:HZ1	1.84	0.42
3:A:4751[C]:FAD:N3A	1:B:37[C]:LYS:HG2	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:402[C]:GLY:HA3	1:C:421[C]:LEU:O	2.19	0.42
1:D:282[C]:PRO:HB3	1:D:321[C]:VAL:HA	2.01	0.42
1:E:281[C]:ARG:H	1:E:281[C]:ARG:HG2	1.52	0.42
1:I:46[C]:LEU:HD21	1:I:100[C]:THR:HG22	2.01	0.42
1:I:208[C]:GLU:OE1	1:I:208[C]:GLU:CA	2.67	0.42
1:I:241[C]:THR:HG22	1:I:260[C]:ALA:CA	2.46	0.42
1:J:388[C]:PHE:C	1:J:390[C]:ALA:N	2.72	0.42
1:A:447[A]:ARG:HH11	1:A:447[A]:ARG:CG	2.32	0.42
1:B:193[A]:LEU:HD12	1:B:193[A]:LEU:N	2.34	0.42
1:D:317[A]:ALA:O	1:D:322[A]:VAL:HG11	2.19	0.42
1:D:467[A]:SER:C	1:D:468[A]:PHE:O	2.57	0.42
1:F:123[A]:GLY:O	1:F:126[A]:GLN:N	2.52	0.42
1:G:255[A]:ASP:OD2	1:G:270[A]:THR:HB	2.19	0.42
1:H:17[A]:GLY:H	1:H:20[A]:VAL:HB	1.84	0.42
1:I:56[A]:LEU:HD12	1:I:56[A]:LEU:HA	1.72	0.42
1:I:214[A]:GLY:O	1:I:218[A]:ILE:CD1	2.68	0.42
1:J:450[A]:HIS:O	1:J:451[A]:ALA:C	2.57	0.42
2:M:134[A]:ALA:O	2:M:137[A]:ASN:HB3	2.19	0.42
2:O:154[A]:PRO:HG2	2:O:157[A]:ILE:HD13	2.01	0.42
1:A:447[C]:ARG:HH11	1:A:447[C]:ARG:CG	2.32	0.42
1:B:193[C]:LEU:HD12	1:B:193[C]:LEU:N	2.34	0.42
1:D:317[C]:ALA:O	1:D:322[C]:VAL:HG11	2.19	0.42
1:D:467[C]:SER:C	1:D:468[C]:PHE:O	2.57	0.42
1:F:123[C]:GLY:O	1:F:126[C]:GLN:N	2.52	0.42
1:G:255[C]:ASP:OD2	1:G:270[C]:THR:HB	2.19	0.42
1:H:17[C]:GLY:H	1:H:20[C]:VAL:HB	1.84	0.42
1:I:56[C]:LEU:HD12	1:I:56[C]:LEU:HA	1.72	0.42
1:I:214[C]:GLY:O	1:I:218[C]:ILE:CD1	2.68	0.42
1:J:450[C]:HIS:O	1:J:451[C]:ALA:C	2.57	0.42
1:A:212[A]:HIS:HE1	1:A:215[A]:GLY:O	2.03	0.42
1:C:123[A]:GLY:O	1:C:125[A]:ASN:N	2.52	0.42
1:C:322[A]:VAL:CG1	1:C:323[A]:ALA:N	2.81	0.42
1:D:369[A]:LYS:CE	1:D:377[A]:GLU:OE2	2.65	0.42
1:D:465[A]:ALA:HB2	1:D:471[A]:SER:HB3	2.02	0.42
1:E:402[A]:GLY:HA3	1:E:421[A]:LEU:O	2.20	0.42
1:F:295[A]:GLU:H	1:F:295[A]:GLU:HG2	1.64	0.42
1:F:312[A]:ILE:HA	1:F:313[A]:PRO:HD3	1.81	0.42
1:F:347[A]:VAL:HG23	1:F:347[A]:VAL:O	2.19	0.42
1:G:15[A]:GLY:HA2	1:G:42[A]:GLY:O	2.19	0.42
1:G:225[A]:ASN:O	1:G:229[A]:ILE:HG12	2.20	0.42
1:G:410[A]:LYS:O	1:G:410[A]:LYS:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:15[A]:GLY:O	1:I:17[A]:GLY:N	2.53	0.42
1:J:44[A]:THR:HG23	4:J:4759[A]:FAD:O1A	2.18	0.42
4:J:4759[A]:FAD:HM83	4:J:4759[A]:FAD:HM71	1.84	0.42
2:N:130[A]:ARG:N	2:N:157[A]:ILE:CG2	2.70	0.42
1:A:212[C]:HIS:HE1	1:A:215[C]:GLY:O	2.03	0.42
1:C:123[C]:GLY:O	1:C:125[C]:ASN:N	2.52	0.42
1:C:322[C]:VAL:CG1	1:C:323[C]:ALA:N	2.81	0.42
1:D:369[C]:LYS:CE	1:D:377[C]:GLU:OE2	2.65	0.42
1:D:465[C]:ALA:HB2	1:D:471[C]:SER:HB3	2.02	0.42
1:E:402[C]:GLY:HA3	1:E:421[C]:LEU:O	2.20	0.42
1:F:295[C]:GLU:H	1:F:295[C]:GLU:HG2	1.64	0.42
1:F:312[C]:ILE:HA	1:F:313[C]:PRO:HD3	1.81	0.42
1:F:347[C]:VAL:HG23	1:F:347[C]:VAL:O	2.19	0.42
1:G:15[C]:GLY:HA2	1:G:42[C]:GLY:O	2.19	0.42
1:G:225[C]:ASN:O	1:G:229[C]:ILE:HG12	2.20	0.42
1:G:410[C]:LYS:O	1:G:410[C]:LYS:HG2	2.19	0.42
1:I:15[C]:GLY:O	1:I:17[C]:GLY:N	2.53	0.42
3:I:4759[C]:FAD:HM83	3:I:4759[C]:FAD:HM71	1.84	0.42
3:I:4759[C]:FAD:O1A	1:J:44[C]:THR:HG23	2.18	0.42
2:M:142[C]:HIS:O	2:M:143[C]:SER:C	2.58	0.42
1:B:329[A]:HIS:CD2	1:B:329[A]:HIS:H	2.37	0.42
1:C:1[A]:ALA:CB	1:C:3[A]:GLN:HE22	2.33	0.42
1:C:123[A]:GLY:O	1:C:124[A]:LYS:C	2.58	0.42
1:C:356[A]:SER:O	1:C:365[A]:ALA:HA	2.20	0.42
1:E:251[A]:ASP:OD1	1:E:251[A]:ASP:C	2.58	0.42
1:E:443[A]:GLU:OE1	2:M:134[A]:ALA:HB1	2.20	0.42
1:F:258[A]:ILE:H	1:F:258[A]:ILE:HG13	1.61	0.42
1:G:274[A]:LEU:HD23	1:G:275[A]:LEU:N	2.35	0.42
1:G:298[A]:PRO:HG2	1:G:299[A]:ARG:HE	1.85	0.42
2:M:162[A]:ASP:O	2:M:163[A]:ALA:C	2.58	0.42
1:B:329[C]:HIS:CD2	1:B:329[C]:HIS:H	2.37	0.42
1:C:1[C]:ALA:CB	1:C:3[C]:GLN:HE22	2.33	0.42
1:C:123[C]:GLY:O	1:C:124[C]:LYS:C	2.58	0.42
1:C:356[C]:SER:O	1:C:365[C]:ALA:HA	2.20	0.42
1:E:251[C]:ASP:OD1	1:E:251[C]:ASP:C	2.58	0.42
1:F:258[C]:ILE:H	1:F:258[C]:ILE:HG13	1.61	0.42
1:G:274[C]:LEU:HD23	1:G:275[C]:LEU:N	2.35	0.42
1:G:298[C]:PRO:HG2	1:G:299[C]:ARG:HE	1.85	0.42
2:K:132[C]:SER:O	2:K:135[C]:ALA:N	2.53	0.42
2:M:159[C]:THR:CG2	2:M:161[C]:GLU:N	2.75	0.42
2:N:142[C]:HIS:CD2	2:N:167[C]:VAL:HG13	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:381[A]:TYR:HA	1:C:408[A]:GLY:O	2.20	0.42
1:D:297[A]:ASP:HB2	1:D:298[A]:PRO:CD	2.47	0.42
1:E:16[A]:PRO:O	1:E:20[A]:VAL:HG13	2.20	0.42
1:H:30[A]:PHE:CE2	1:H:343[A]:ALA:HB2	2.55	0.42
1:I:121[A]:ILE:O	1:I:121[A]:ILE:HG12	2.20	0.42
2:K:155[A]:ARG:HH12	2:K:157[A]:ILE:HD11	1.84	0.42
1:C:381[C]:TYR:HA	1:C:408[C]:GLY:O	2.20	0.42
1:D:297[C]:ASP:HB2	1:D:298[C]:PRO:CD	2.47	0.42
1:D:414[C]:ARG:CD	2:L:161[C]:GLU:OE2	2.64	0.42
1:E:16[C]:PRO:O	1:E:20[C]:VAL:HG13	2.20	0.42
1:H:30[C]:PHE:CE2	1:H:343[C]:ALA:HB2	2.55	0.42
1:I:121[C]:ILE:O	1:I:121[C]:ILE:HG12	2.20	0.42
1:A:397[A]:ASN:N	1:A:397[A]:ASN:ND2	2.68	0.42
1:C:353[A]:CYS:CB	1:C:437[A]:GLU:OE1	2.67	0.42
1:D:221[A]:GLU:HG2	1:D:225[A]:ASN:HD21	1.84	0.42
1:D:275[A]:LEU:CD2	1:D:275[A]:LEU:C	2.87	0.42
1:D:288[A]:GLY:O	1:D:292[A]:LEU:HD12	2.20	0.42
1:E:281[A]:ARG:HA	1:E:282[A]:PRO:HD3	1.88	0.42
1:E:395[A]:LYS:HG2	1:F:99[A]:LEU:HG	2.01	0.42
1:H:287[A]:LEU:HB3	4:H:4807[A]:HOH:O	2.19	0.42
1:I:174[A]:LEU:HD12	1:I:197[A]:TRP:CE2	2.55	0.42
1:I:220[A]:MET:O	1:I:221[A]:GLU:C	2.57	0.42
1:J:234[A]:GLY:O	1:J:236[A]:LYS:HD3	2.20	0.42
1:J:327[A]:LEU:CA	4:J:4759[A]:FAD:O3'	2.68	0.42
1:J:393[A]:ARG:NH1	1:J:393[A]:ARG:HG2	2.35	0.42
1:A:397[C]:ASN:ND2	1:A:397[C]:ASN:N	2.68	0.42
1:C:353[C]:CYS:CB	1:C:437[C]:GLU:OE1	2.67	0.42
1:D:221[C]:GLU:HG2	1:D:225[C]:ASN:HD21	1.84	0.42
1:D:275[C]:LEU:CD2	1:D:275[C]:LEU:C	2.87	0.42
1:D:288[C]:GLY:O	1:D:292[C]:LEU:HD12	2.20	0.42
1:E:281[C]:ARG:HA	1:E:282[C]:PRO:HD3	1.88	0.42
1:E:395[C]:LYS:HG2	1:F:99[C]:LEU:HG	2.01	0.42
4:G:4807[C]:HOH:O	1:H:287[C]:LEU:HB3	2.19	0.42
1:I:174[C]:LEU:HD12	1:I:197[C]:TRP:CE2	2.55	0.42
1:I:220[C]:MET:O	1:I:221[C]:GLU:C	2.57	0.42
3:I:4759[C]:FAD:O3'	1:J:327[C]:LEU:CA	2.68	0.42
1:J:234[C]:GLY:O	1:J:236[C]:LYS:HD3	2.20	0.42
1:J:393[C]:ARG:NH1	1:J:393[C]:ARG:HG2	2.35	0.42
1:B:409[A]:GLN:HE21	1:B:409[A]:GLN:HB2	1.52	0.42
1:D:374[A]:LEU:HD12	1:D:374[A]:LEU:HA	1.91	0.42
1:E:131[A]:LYS:HZ2	1:E:132[A]:ALA:H	1.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:188[A]:VAL:O	1:E:192[A]:GLU:HG3	2.20	0.42
1:E:304[A]:VAL:HG11	1:E:317[A]:ALA:HB3	2.02	0.42
1:H:164[A]:THR:HB	1:H:254[A]:ILE:HD11	2.02	0.42
1:I:146[A]:ILE:HD12	1:I:317[A]:ALA:HB2	2.02	0.42
1:I:209[A]:PHE:HA	1:I:241[A]:THR:O	2.20	0.42
1:I:448[A]:VAL:HG11	1:J:434[A]:LEU:HA	2.01	0.42
1:J:209[A]:PHE:HA	1:J:241[A]:THR:O	2.20	0.42
2:K:142[A]:HIS:O	2:K:144[A]:LEU:N	2.53	0.42
2:M:135[A]:ALA:O	2:M:138[A]:ILE:HG12	2.19	0.42
1:B:409[C]:GLN:HE21	1:B:409[C]:GLN:HB2	1.52	0.42
1:D:374[C]:LEU:HD12	1:D:374[C]:LEU:HA	1.91	0.42
1:E:131[C]:LYS:HZ2	1:E:132[C]:ALA:H	1.68	0.42
1:E:188[C]:VAL:O	1:E:192[C]:GLU:HG3	2.20	0.42
1:E:304[C]:VAL:HG11	1:E:317[C]:ALA:HB3	2.02	0.42
1:H:164[C]:THR:HB	1:H:254[C]:ILE:HD11	2.02	0.42
1:I:146[C]:ILE:HD12	1:I:317[C]:ALA:HB2	2.02	0.42
1:I:209[C]:PHE:HA	1:I:241[C]:THR:O	2.20	0.42
1:I:448[C]:VAL:HG11	1:J:434[C]:LEU:HA	2.01	0.42
1:J:209[C]:PHE:HA	1:J:241[C]:THR:O	2.20	0.42
2:K:132[C]:SER:C	2:K:134[C]:ALA:N	2.73	0.42
1:A:198[A]:GLN:CB	1:A:204[A]:VAL:HG21	2.50	0.41
1:A:269[A]:ILE:HG22	1:A:270[A]:THR:N	2.35	0.41
1:B:92[A]:LYS:HE2	1:B:92[A]:LYS:HB3	1.90	0.41
1:B:325[A]:PRO:HB2	1:B:327[A]:LEU:HD12	2.02	0.41
1:C:137[A]:GLN:NE2	1:C:137[A]:GLN:HA	2.34	0.41
1:C:320[A]:ASP:CB	1:C:326[A]:MET:HG2	2.50	0.41
1:D:262[A]:SER:O	1:D:263[A]:GLY:O	2.37	0.41
1:D:275[A]:LEU:HD23	1:D:276[A]:VAL:H	1.84	0.41
1:G:220[A]:MET:CE	1:G:224[A]:LYS:HE3	2.49	0.41
1:G:299[A]:ARG:HH11	1:G:299[A]:ARG:CG	2.31	0.41
1:H:118[A]:TYR:OH	1:H:285[A]:LYS:O	2.24	0.41
1:J:224[A]:LYS:HA	1:J:224[A]:LYS:HD3	1.92	0.41
1:J:444[A]:ASP:OD1	2:O:155[A]:ARG:HG3	2.19	0.41
2:L:157[A]:ILE:CG2	2:L:158[A]:PHE:N	2.82	0.41
1:A:198[C]:GLN:CB	1:A:204[C]:VAL:HG21	2.50	0.41
1:A:269[C]:ILE:HG22	1:A:270[C]:THR:N	2.35	0.41
1:B:92[C]:LYS:HE2	1:B:92[C]:LYS:HB3	1.90	0.41
1:B:325[C]:PRO:HB2	1:B:327[C]:LEU:HD12	2.02	0.41
1:C:137[C]:GLN:NE2	1:C:137[C]:GLN:HA	2.34	0.41
1:C:320[C]:ASP:CB	1:C:326[C]:MET:HG2	2.50	0.41
1:D:262[C]:SER:O	1:D:263[C]:GLY:O	2.37	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:275[C]:LEU:HD23	1:D:276[C]:VAL:H	1.84	0.41
1:G:220[C]:MET:CE	1:G:224[C]:LYS:HE3	2.49	0.41
1:G:299[C]:ARG:HH11	1:G:299[C]:ARG:CG	2.31	0.41
1:H:118[C]:TYR:OH	1:H:285[C]:LYS:O	2.24	0.41
1:J:224[C]:LYS:HA	1:J:224[C]:LYS:HD3	1.92	0.41
1:A:375[A]:LYS:C	1:A:377[A]:GLU:N	2.73	0.41
1:A:454[A]:THR:HB	1:B:427[A]:GLU:OE2	2.20	0.41
1:B:24[A]:LYS:HG3	1:B:339[A]:VAL:CG2	2.49	0.41
1:D:224[A]:LYS:HZ2	1:D:224[A]:LYS:HG2	1.53	0.41
1:F:161[A]:ASP:OD1	1:F:163[A]:ASP:HB3	2.19	0.41
1:F:440[A]:ALA:HA	2:M:155[A]:ARG:HH12	1.83	0.41
1:G:20[A]:VAL:HG23	1:G:336[A]:ILE:HD12	2.00	0.41
1:H:10[A]:THR:CG2	1:H:139[A]:ILE:HG21	2.46	0.41
1:H:91[A]:GLN:HE21	1:H:91[A]:GLN:HB2	1.50	0.41
2:K:164[A]:LEU:O	2:K:167[A]:VAL:HB	2.20	0.41
1:A:375[C]:LYS:C	1:A:377[C]:GLU:N	2.73	0.41
1:A:454[C]:THR:HB	1:B:427[C]:GLU:OE2	2.20	0.41
1:B:24[C]:LYS:HG3	1:B:339[C]:VAL:CG2	2.49	0.41
1:D:224[C]:LYS:HZ2	1:D:224[C]:LYS:HG2	1.53	0.41
1:F:161[C]:ASP:OD1	1:F:163[C]:ASP:HB3	2.19	0.41
1:G:20[C]:VAL:HG23	1:G:336[C]:ILE:HD12	2.00	0.41
1:H:10[C]:THR:CG2	1:H:139[C]:ILE:HG21	2.46	0.41
1:H:91[C]:GLN:HE21	1:H:91[C]:GLN:HB2	1.50	0.41
1:A:145[A]:LEU:HD21	1:A:318[A]:ILE:HG13	2.02	0.41
1:A:219[A]:ASP:OD2	1:A:221[A]:GLU:HB3	2.19	0.41
1:A:282[A]:PRO:HB3	1:A:321[A]:VAL:HA	2.02	0.41
1:A:412[A]:THR:HG22	2:K:161[A]:GLU:HG3	2.03	0.41
1:C:307[A]:ARG:HB2	1:C:309[A]:GLN:HE21	1.86	0.41
1:D:44[A]:THR:HG23	3:D:4753[A]:FAD:PA	2.60	0.41
1:D:220[A]:MET:CE	1:D:220[A]:MET:CG	2.96	0.41
1:G:318[A]:ILE:HG21	1:G:318[A]:ILE:HD13	1.62	0.41
1:H:148[A]:THR:HG22	3:H:4757[A]:FAD:N7A	2.35	0.41
1:A:145[C]:LEU:HD21	1:A:318[C]:ILE:HG13	2.02	0.41
1:A:219[C]:ASP:OD2	1:A:221[C]:GLU:HB3	2.19	0.41
1:A:282[C]:PRO:HB3	1:A:321[C]:VAL:HA	2.02	0.41
1:C:307[C]:ARG:HB2	1:C:309[C]:GLN:HE21	1.86	0.41
3:C:4753[C]:FAD:PA	1:D:44[C]:THR:HG23	2.60	0.41
1:D:220[C]:MET:CE	1:D:220[C]:MET:CG	2.96	0.41
1:G:318[C]:ILE:HG21	1:G:318[C]:ILE:HD13	1.62	0.41
3:G:4757[C]:FAD:N7A	1:H:148[C]:THR:HG22	2.35	0.41
1:B:137[A]:GLN:NE2	1:B:138[A]:VAL:H	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:167[A]:SER:OG	1:C:169[A]:THR:HG23	2.21	0.41
1:C:200[A]:LEU:HD12	1:C:200[A]:LEU:HA	1.71	0.41
1:F:49[A]:GLY:HA2	3:F:4755[A]:FAD:HM82	2.03	0.41
1:F:178[A]:PRO:HB3	1:F:273[A]:VAL:CG2	2.50	0.41
1:F:230[A]:LEU:HD23	1:F:230[A]:LEU:HA	1.88	0.41
1:F:456[A]:SER:O	1:F:459[A]:PHE:HB3	2.20	0.41
1:G:35[A]:ILE:HD12	1:G:35[A]:ILE:H	1.85	0.41
1:G:239[A]:LEU:HD12	1:G:239[A]:LEU:N	2.33	0.41
1:H:385[A]:LYS:HG2	1:H:403[A]:MET:CE	2.50	0.41
1:H:448[A]:VAL:O	1:H:450[A]:HIS:HD2	2.03	0.41
1:I:432[A]:ALA:O	1:I:436[A]:LEU:HB2	2.21	0.41
2:K:155[A]:ARG:O	2:K:156[A]:GLY:C	2.58	0.41
1:B:137[C]:GLN:NE2	1:B:138[C]:VAL:H	2.18	0.41
1:C:167[C]:SER:OG	1:C:169[C]:THR:HG23	2.21	0.41
1:C:200[C]:LEU:HD12	1:C:200[C]:LEU:HA	1.71	0.41
3:E:4755[C]:FAD:HM82	1:F:49[C]:GLY:HA2	2.03	0.41
1:F:178[C]:PRO:HB3	1:F:273[C]:VAL:CG2	2.50	0.41
1:F:230[C]:LEU:HD23	1:F:230[C]:LEU:HA	1.88	0.41
1:F:456[C]:SER:O	1:F:459[C]:PHE:HB3	2.20	0.41
1:G:35[C]:ILE:HD12	1:G:35[C]:ILE:H	1.85	0.41
1:G:239[C]:LEU:HD12	1:G:239[C]:LEU:N	2.33	0.41
1:H:385[C]:LYS:HG2	1:H:403[C]:MET:CE	2.50	0.41
1:H:448[C]:VAL:O	1:H:450[C]:HIS:HD2	2.03	0.41
1:I:432[C]:ALA:O	1:I:436[C]:LEU:HB2	2.21	0.41
1:A:221[A]:GLU:HB3	1:A:405[A]:LYS:NZ	2.36	0.41
1:B:9[A]:VAL:O	1:B:9[A]:VAL:CG2	2.68	0.41
1:B:45[A]:CYS:HG	1:B:50[A]:CYS:HB2	1.83	0.41
1:B:102[A]:GLY:O	1:B:106[A]:LEU:HG	2.20	0.41
1:B:301[A]:ARG:HB3	1:B:322[A]:VAL:HA	2.01	0.41
1:D:326[A]:MET:CE	1:D:326[A]:MET:CG	2.94	0.41
1:E:321[A]:VAL:CG1	1:E:322[A]:VAL:HG23	2.48	0.41
1:F:182[A]:VAL:HG23	1:F:271[A]:CYS:HB3	2.03	0.41
1:G:290[A]:GLU:OE1	1:G:290[A]:GLU:HA	2.20	0.41
1:I:154[A]:PRO:O	1:I:156[A]:PRO:HD3	2.20	0.41
1:I:155[A]:PHE:HZ	1:I:243[A]:VAL:HG23	1.81	0.41
1:I:222[A]:ILE:HD13	1:I:419[A]:HIS:HB3	2.01	0.41
1:A:221[C]:GLU:HB3	1:A:405[C]:LYS:NZ	2.36	0.41
1:B:9[C]:VAL:O	1:B:9[C]:VAL:CG2	2.68	0.41
1:B:45[C]:CYS:HG	1:B:50[C]:CYS:HB2	1.83	0.41
1:B:102[C]:GLY:O	1:B:106[C]:LEU:HG	2.20	0.41
1:B:301[C]:ARG:HB3	1:B:322[C]:VAL:HA	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:326[C]:MET:CE	1:D:326[C]:MET:CG	2.94	0.41
1:E:321[C]:VAL:CG1	1:E:322[C]:VAL:HG23	2.48	0.41
1:F:182[C]:VAL:HG23	1:F:271[C]:CYS:HB3	2.03	0.41
1:G:290[C]:GLU:HA	1:G:290[C]:GLU:OE1	2.20	0.41
1:I:154[C]:PRO:O	1:I:156[C]:PRO:HD3	2.20	0.41
1:I:155[C]:PHE:HZ	1:I:243[C]:VAL:HG23	1.81	0.41
1:I:222[C]:ILE:HD13	1:I:419[C]:HIS:HB3	2.01	0.41
2:L:153[C]:GLY:HA3	2:L:157[C]:ILE:O	2.21	0.41
1:A:256[A]:VAL:HG22	1:A:269[A]:ILE:HB	2.01	0.41
1:C:1[A]:ALA:HB1	1:C:3[A]:GLN:HE22	1.84	0.41
1:C:270[A]:THR:HG22	1:C:271[A]:CYS:N	2.35	0.41
1:C:354[A]:VAL:HA	1:C:355[A]:PRO:HD3	1.89	0.41
1:D:277[A]:CYS:HB2	4:D:4789[A]:HOH:O	2.19	0.41
1:E:16[A]:PRO:CG	1:E:45[A]:CYS:HB2	2.51	0.41
1:E:336[A]:ILE:HG22	1:E:337[A]:ILE:N	2.34	0.41
1:F:154[A]:PRO:CD	1:F:281[A]:ARG:NH2	2.83	0.41
1:F:330[A]:LYS:O	1:F:331[A]:ALA:C	2.59	0.41
1:F:386[A]:PHE:CD2	1:F:461[A]:GLU:HB3	2.55	0.41
1:G:15[A]:GLY:HA2	1:G:42[A]:GLY:C	2.41	0.41
1:G:452[A]:HIS:HA	1:G:453[A]:PRO:HA	1.82	0.41
1:I:2[A]:ASP:HB2	4:I:4773[A]:HOH:O	2.20	0.41
1:I:325[A]:PRO:O	1:I:330[A]:LYS:HD2	2.21	0.41
1:I:368[A]:GLY:HA3	1:I:417[A]:GLY:HA2	2.02	0.41
1:A:256[C]:VAL:HG22	1:A:269[C]:ILE:HB	2.01	0.41
1:C:1[C]:ALA:HB1	1:C:3[C]:GLN:HE22	1.84	0.41
1:C:270[C]:THR:HG22	1:C:271[C]:CYS:N	2.35	0.41
1:C:354[C]:VAL:HA	1:C:355[C]:PRO:HD3	1.89	0.41
4:C:4789[C]:HOH:O	1:D:277[C]:CYS:HB2	2.19	0.41
1:E:16[C]:PRO:CG	1:E:45[C]:CYS:HB2	2.51	0.41
1:E:336[C]:ILE:HG22	1:E:337[C]:ILE:N	2.34	0.41
1:F:154[C]:PRO:CD	1:F:281[C]:ARG:NH2	2.83	0.41
1:F:330[C]:LYS:O	1:F:331[C]:ALA:C	2.59	0.41
1:F:386[C]:PHE:CD2	1:F:461[C]:GLU:HB3	2.55	0.41
1:G:15[C]:GLY:HA2	1:G:42[C]:GLY:C	2.41	0.41
1:G:452[C]:HIS:HA	1:G:453[C]:PRO:HA	1.82	0.41
4:H:4773[C]:HOH:O	1:I:2[C]:ASP:HB2	2.20	0.41
1:I:325[C]:PRO:O	1:I:330[C]:LYS:HD2	2.21	0.41
1:I:368[C]:GLY:HA3	1:I:417[C]:GLY:HA2	2.02	0.41
1:A:172[A]:LEU:HD23	1:A:172[A]:LEU:HA	1.77	0.41
1:B:46[A]:LEU:HG	1:B:100[A]:THR:HG22	2.02	0.41
1:B:182[A]:VAL:HG23	1:B:271[A]:CYS:CB	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:193[A]:LEU:N	1:C:193[A]:LEU:HD12	2.35	0.41
1:C:230[A]:LEU:HA	1:C:230[A]:LEU:HD12	1.85	0.41
3:C:4752[A]:FAD:H9	3:C:4752[A]:FAD:H1'1	1.92	0.41
1:D:191[A]:VAL:O	1:D:192[A]:GLU:C	2.59	0.41
1:D:192[A]:GLU:O	1:D:196[A]:VAL:HG23	2.21	0.41
1:D:409[A]:GLN:NE2	1:D:411[A]:SER:H	1.92	0.41
1:E:464[A]:LEU:HD22	1:E:470[A]:LYS:O	2.21	0.41
1:F:69[A]:LYS:H	1:F:69[A]:LYS:HG2	1.52	0.41
1:F:208[A]:GLU:OE1	1:F:209[A]:PHE:N	2.51	0.41
1:F:319[A]:GLY:O	1:F:322[A]:VAL:HG22	2.21	0.41
1:H:15[A]:GLY:O	1:H:16[A]:PRO:C	2.59	0.41
1:H:89[A]:MET:O	1:H:92[A]:LYS:HB3	2.19	0.41
1:H:242[A]:LYS:HG3	1:H:259[A]:GLU:O	2.21	0.41
1:H:290[A]:GLU:CD	1:H:290[A]:GLU:N	2.70	0.41
1:I:87[A]:LYS:HD2	1:J:72[A]:ALA:O	2.21	0.41
1:J:337[A]:ILE:O	1:J:347[A]:VAL:HG12	2.20	0.41
2:M:168[A]:GLN:HA	2:M:171[A]:GLN:HG2	2.02	0.41
1:A:172[C]:LEU:HD23	1:A:172[C]:LEU:HA	1.77	0.41
1:B:46[C]:LEU:HG	1:B:100[C]:THR:HG22	2.02	0.41
1:B:182[C]:VAL:HG23	1:B:271[C]:CYS:CB	2.51	0.41
3:B:4752[C]:FAD:H9	3:B:4752[C]:FAD:H1'1	1.92	0.41
1:C:193[C]:LEU:N	1:C:193[C]:LEU:HD12	2.35	0.41
1:C:230[C]:LEU:HA	1:C:230[C]:LEU:HD12	1.85	0.41
1:D:191[C]:VAL:O	1:D:192[C]:GLU:C	2.59	0.41
1:D:192[C]:GLU:O	1:D:196[C]:VAL:HG23	2.21	0.41
1:D:409[C]:GLN:NE2	1:D:411[C]:SER:H	1.92	0.41
1:E:464[C]:LEU:HD22	1:E:470[C]:LYS:O	2.21	0.41
1:F:69[C]:LYS:H	1:F:69[C]:LYS:HG2	1.52	0.41
1:F:208[C]:GLU:OE1	1:F:209[C]:PHE:N	2.51	0.41
1:F:319[C]:GLY:O	1:F:322[C]:VAL:HG22	2.21	0.41
1:H:15[C]:GLY:O	1:H:16[C]:PRO:C	2.59	0.41
1:H:89[C]:MET:O	1:H:92[C]:LYS:HB3	2.19	0.41
1:H:242[C]:LYS:HG3	1:H:259[C]:GLU:O	2.21	0.41
1:H:290[C]:GLU:CD	1:H:290[C]:GLU:N	2.70	0.41
1:I:87[C]:LYS:HD2	1:J:72[C]:ALA:O	2.21	0.41
1:J:337[C]:ILE:O	1:J:347[C]:VAL:HG12	2.20	0.41
2:N:135[C]:ALA:O	2:N:136[C]:ARG:C	2.58	0.41
1:A:6[A]:ASP:O	1:A:31[A]:LYS:HD3	2.20	0.41
1:A:74[A]:ARG:HE	1:B:59[A]:ASN:ND2	2.19	0.41
1:A:171[A]:ALA:HA	1:A:174[A]:LEU:HD22	2.03	0.41
1:C:302[A]:ILE:HG21	1:C:302[A]:ILE:HD13	1.70	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:6[A]:ASP:O	1:D:31[A]:LYS:HD3	2.20	0.41
1:E:306[A]:THR:O	1:E:306[A]:THR:CG2	2.66	0.41
1:F:30[A]:PHE:O	1:F:32[A]:THR:HG23	2.20	0.41
1:G:91[A]:GLN:O	1:G:94[A]:THR:HB	2.21	0.41
1:I:33[A]:VAL:CA	1:I:113[A]:VAL:HG23	2.48	0.41
1:J:184[A]:ILE:HD12	1:J:243[A]:VAL:HG11	2.03	0.41
1:J:330[A]:LYS:O	1:J:334[A]:GLU:HB2	2.20	0.41
1:A:6[C]:ASP:O	1:A:31[C]:LYS:HD3	2.20	0.41
1:A:74[C]:ARG:HE	1:B:59[C]:ASN:ND2	2.19	0.41
1:A:171[C]:ALA:HA	1:A:174[C]:LEU:HD22	2.03	0.41
1:C:302[C]:ILE:HG21	1:C:302[C]:ILE:HD13	1.70	0.41
1:D:6[C]:ASP:O	1:D:31[C]:LYS:HD3	2.20	0.41
1:E:306[C]:THR:O	1:E:306[C]:THR:CG2	2.66	0.41
1:F:30[C]:PHE:O	1:F:32[C]:THR:HG23	2.20	0.41
1:G:91[C]:GLN:O	1:G:94[C]:THR:HB	2.21	0.41
1:I:33[C]:VAL:CA	1:I:113[C]:VAL:HG23	2.48	0.41
1:J:184[C]:ILE:HD12	1:J:243[C]:VAL:HG11	2.03	0.41
1:J:330[C]:LYS:O	1:J:334[C]:GLU:HB2	2.20	0.41
1:A:224[A]:LYS:HD3	4:A:4761[A]:HOH:O	2.21	0.41
1:A:302[A]:ILE:HA	1:A:303[A]:PRO:HD2	1.73	0.41
1:B:24[A]:LYS:HG3	1:B:339[A]:VAL:HG21	2.03	0.41
1:B:305[A]:ASN:ND2	1:B:305[A]:ASN:C	2.73	0.41
1:B:426[A]:GLY:O	1:B:429[A]:VAL:HG12	2.21	0.41
1:C:54[A]:LYS:HE3	1:C:57[A]:LEU:HD12	2.03	0.41
1:C:85[A]:LEU:HD12	1:C:176[A]:LYS:HA	2.02	0.41
1:C:452[A]:HIS:CD2	1:C:453[A]:PRO:CB	3.02	0.41
1:C:452[A]:HIS:HA	1:C:453[A]:PRO:HA	1.62	0.41
1:D:10[A]:THR:OG1	1:D:141[A]:THR:HG21	2.21	0.41
1:D:35[A]:ILE:HD11	1:D:139[A]:ILE:CD1	2.44	0.41
1:D:200[A]:LEU:HD12	1:D:200[A]:LEU:HA	1.88	0.41
1:E:303[A]:PRO:HG2	4:E:4773[A]:HOH:O	2.21	0.41
1:F:145[A]:LEU:HD13	1:F:316[A]:TYR:HB2	2.03	0.41
1:F:402[A]:GLY:HA3	1:F:421[A]:LEU:O	2.20	0.41
1:G:155[A]:PHE:HZ	1:G:243[A]:VAL:HG13	1.84	0.41
1:I:121[A]:ILE:HB	1:I:127[A]:VAL:HG12	2.03	0.41
1:I:123[A]:GLY:O	1:I:124[A]:LYS:C	2.58	0.41
1:I:297[A]:ASP:CG	1:I:301[A]:ARG:HG3	2.38	0.41
1:I:455[A]:LEU:HD12	1:I:455[A]:LEU:HA	1.93	0.41
1:J:263[A]:GLY:HA3	1:J:265[A]:LYS:HZ3	1.85	0.41
1:J:349[A]:ILE:HG12	1:J:351[A]:TYR:CD1	2.55	0.41
2:K:159[A]:THR:CG2	2:K:161[A]:GLU:HB2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:135[A]:ALA:O	2:M:136[A]:ARG:C	2.58	0.41
2:N:152[A]:THR:HG22	2:N:153[A]:GLY:N	2.35	0.41
2:N:167[A]:VAL:O	2:N:168[A]:GLN:C	2.60	0.41
1:A:224[C]:LYS:HD3	4:J:4761[C]:HOH:O	2.21	0.41
1:A:302[C]:ILE:HA	1:A:303[C]:PRO:HD2	1.73	0.41
1:B:24[C]:LYS:HG3	1:B:339[C]:VAL:HG21	2.03	0.41
1:B:305[C]:ASN:ND2	1:B:305[C]:ASN:C	2.73	0.41
1:B:426[C]:GLY:O	1:B:429[C]:VAL:HG12	2.21	0.41
1:C:54[C]:LYS:HE3	1:C:57[C]:LEU:HD12	2.03	0.41
1:C:85[C]:LEU:HD12	1:C:176[C]:LYS:HA	2.02	0.41
1:C:452[C]:HIS:CD2	1:C:453[C]:PRO:CB	3.02	0.41
1:C:452[C]:HIS:HA	1:C:453[C]:PRO:HA	1.62	0.41
1:D:10[C]:THR:OG1	1:D:141[C]:THR:HG21	2.21	0.41
1:D:35[C]:ILE:HD11	1:D:139[C]:ILE:CD1	2.44	0.41
1:D:200[C]:LEU:HD12	1:D:200[C]:LEU:HA	1.88	0.41
4:D:4773[C]:HOH:O	1:E:303[C]:PRO:HG2	2.21	0.41
1:F:145[C]:LEU:HD13	1:F:316[C]:TYR:HB2	2.03	0.41
1:F:402[C]:GLY:HA3	1:F:421[C]:LEU:O	2.20	0.41
1:G:155[C]:PHE:HZ	1:G:243[C]:VAL:HG13	1.84	0.41
1:G:437[C]:GLU:CG	2:N:133[C]:PRO:HG3	2.51	0.41
1:I:121[C]:ILE:HB	1:I:127[C]:VAL:HG12	2.03	0.41
1:I:123[C]:GLY:O	1:I:124[C]:LYS:C	2.58	0.41
1:I:297[C]:ASP:CG	1:I:301[C]:ARG:HG3	2.38	0.41
1:I:455[C]:LEU:HD12	1:I:455[C]:LEU:HA	1.93	0.41
1:J:263[C]:GLY:HA3	1:J:265[C]:LYS:HZ3	1.85	0.41
1:J:349[C]:ILE:HG12	1:J:351[C]:TYR:CD1	2.55	0.41
2:K:130[C]:ARG:HD3	2:K:131[C]:LEU:CD2	2.47	0.41
2:K:158[C]:PHE:CZ	2:K:166[C]:LEU:HD23	2.55	0.41
2:M:135[C]:ALA:HB2	2:M:160[C]:LYS:HA	2.03	0.41
2:M:144[C]:LEU:HD23	2:M:148[C]:GLN:HE22	1.86	0.41
1:A:106[A]:LEU:HD11	1:B:473[A]:ASN:HA	2.02	0.41
1:A:154[A]:PRO:HD3	1:A:281[A]:ARG:CZ	2.51	0.41
1:D:26[A]:ALA:HB2	1:D:112[A]:VAL:HG23	2.03	0.41
1:D:259[A]:GLU:O	1:D:260[A]:ALA:C	2.59	0.41
1:D:278[A]:ILE:HG21	1:D:278[A]:ILE:HD13	1.82	0.41
1:E:42[A]:GLY:HA3	1:E:46[A]:LEU:HD23	2.01	0.41
1:G:175[A]:LYS:O	1:G:176[A]:LYS:HB3	2.21	0.41
1:I:138[A]:VAL:O	1:I:139[A]:ILE:HD12	2.20	0.41
1:I:239[A]:LEU:HD23	1:I:239[A]:LEU:HA	1.93	0.41
1:A:106[C]:LEU:HD11	1:B:473[C]:ASN:HA	2.02	0.41
1:A:154[C]:PRO:HD3	1:A:281[C]:ARG:CZ	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:26[C]:ALA:HB2	1:D:112[C]:VAL:HG23	2.03	0.41
1:D:259[C]:GLU:O	1:D:260[C]:ALA:C	2.59	0.41
1:D:278[C]:ILE:HG21	1:D:278[C]:ILE:HD13	1.82	0.41
1:E:42[C]:GLY:HA3	1:E:46[C]:LEU:HD23	2.01	0.41
1:G:175[C]:LYS:O	1:G:176[C]:LYS:HB3	2.21	0.41
1:I:138[C]:VAL:O	1:I:139[C]:ILE:HD12	2.20	0.41
1:I:239[C]:LEU:HD23	1:I:239[C]:LEU:HA	1.93	0.41
1:A:55[A]:ALA:HB2	1:B:396[A]:THR:OG1	2.21	0.40
1:A:210[A]:LEU:HD22	1:A:210[A]:LEU:N	2.35	0.40
1:B:16[A]:PRO:O	1:B:18[A]:GLY:N	2.54	0.40
1:B:452[A]:HIS:CD2	1:B:453[A]:PRO:CA	3.04	0.40
1:C:182[A]:VAL:O	1:C:274[A]:LEU:HD12	2.20	0.40
1:C:320[A]:ASP:OD1	4:C:4755[A]:HOH:O	2.21	0.40
1:E:379[A]:ILE:HD13	1:E:379[A]:ILE:HG21	1.75	0.40
1:G:83[A]:LEU:O	1:G:83[A]:LEU:HG	2.18	0.40
1:G:149[A]:GLY:HA2	1:G:320[A]:ASP:HB2	2.02	0.40
1:G:448[A]:VAL:O	1:G:460[A]:ARG:CZ	2.69	0.40
1:I:275[A]:LEU:HD22	1:I:275[A]:LEU:C	2.41	0.40
1:J:116[A]:ASN:O	1:J:131[A]:LYS:HG2	2.21	0.40
1:J:287[A]:LEU:HD12	1:J:287[A]:LEU:HA	1.91	0.40
1:J:406[A]:ILE:O	1:J:406[A]:ILE:HG12	2.20	0.40
1:J:436[A]:LEU:HA	1:J:436[A]:LEU:HD22	1.78	0.40
2:M:152[A]:THR:CG2	2:M:153[A]:GLY:H	2.33	0.40
1:A:55[C]:ALA:HB2	1:B:396[C]:THR:OG1	2.21	0.40
1:A:210[C]:LEU:HD22	1:A:210[C]:LEU:N	2.35	0.40
1:B:16[C]:PRO:O	1:B:18[C]:GLY:N	2.54	0.40
1:B:452[C]:HIS:CD2	1:B:453[C]:PRO:CA	3.04	0.40
4:B:4755[C]:HOH:O	1:C:320[C]:ASP:OD1	2.21	0.40
1:C:182[C]:VAL:O	1:C:274[C]:LEU:HD12	2.20	0.40
1:E:379[C]:ILE:HD13	1:E:379[C]:ILE:HG21	1.75	0.40
1:G:83[C]:LEU:O	1:G:83[C]:LEU:HG	2.18	0.40
1:G:149[C]:GLY:HA2	1:G:320[C]:ASP:HB2	2.02	0.40
1:G:448[C]:VAL:O	1:G:460[C]:ARG:CZ	2.69	0.40
1:I:275[C]:LEU:HD22	1:I:275[C]:LEU:C	2.41	0.40
1:J:116[C]:ASN:O	1:J:131[C]:LYS:HG2	2.21	0.40
1:J:287[C]:LEU:HD12	1:J:287[C]:LEU:HA	1.91	0.40
1:J:406[C]:ILE:O	1:J:406[C]:ILE:HG12	2.20	0.40
1:J:436[C]:LEU:HA	1:J:436[C]:LEU:HD22	1.78	0.40
1:A:146[A]:ILE:HG23	1:A:148[A]:THR:HG23	2.03	0.40
1:B:55[A]:ALA:HB3	1:B:92[A]:LYS:HG3	2.03	0.40
1:B:361[A]:HIS:HA	1:B:362[A]:PRO:C	2.40	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:51[A]:ILE:N	1:C:52[A]:PRO:CD	2.84	0.40
1:C:318[A]:ILE:CD1	1:C:335[A]:GLY:HA2	2.52	0.40
1:E:256[A]:VAL:HG22	1:E:269[A]:ILE:HB	2.02	0.40
1:F:85[A]:LEU:HA	1:F:85[A]:LEU:HD12	1.88	0.40
1:F:464[A]:LEU:HD21	1:F:472[A]:ILE:CD1	2.52	0.40
1:G:107[A]:PHE:HD1	1:G:107[A]:PHE:HA	1.76	0.40
1:G:320[A]:ASP:HB3	1:G:326[A]:MET:CE	2.52	0.40
1:H:167[A]:SER:O	1:H:168[A]:SER:C	2.59	0.40
1:I:85[A]:LEU:HD22	1:I:89[A]:MET:HG2	2.03	0.40
1:I:291[A]:GLU:O	1:I:292[A]:LEU:CD1	2.68	0.40
1:I:406[A]:ILE:HG23	1:I:466[A]:ALA:HB2	2.04	0.40
1:J:59[A]:ASN:N	1:J:59[A]:ASN:ND2	2.68	0.40
1:J:122[A]:THR:OG1	1:J:128[A]:THR:HG22	2.22	0.40
1:J:448[A]:VAL:HG12	1:J:449[A]:CYS:N	2.35	0.40
1:A:146[C]:ILE:HG23	1:A:148[C]:THR:HG23	2.03	0.40
1:B:55[C]:ALA:HB3	1:B:92[C]:LYS:HG3	2.03	0.40
1:B:361[C]:HIS:HA	1:B:362[C]:PRO:C	2.40	0.40
1:C:51[C]:ILE:N	1:C:52[C]:PRO:CD	2.84	0.40
1:C:318[C]:ILE:CD1	1:C:335[C]:GLY:HA2	2.52	0.40
1:E:256[C]:VAL:HG22	1:E:269[C]:ILE:HB	2.02	0.40
1:F:85[C]:LEU:HA	1:F:85[C]:LEU:HD12	1.88	0.40
1:F:464[C]:LEU:HD21	1:F:472[C]:ILE:CD1	2.52	0.40
1:G:107[C]:PHE:HD1	1:G:107[C]:PHE:HA	1.76	0.40
1:G:320[C]:ASP:HB3	1:G:326[C]:MET:CE	2.52	0.40
1:H:167[C]:SER:O	1:H:168[C]:SER:C	2.59	0.40
1:I:85[C]:LEU:HD22	1:I:89[C]:MET:HG2	2.03	0.40
1:I:291[C]:GLU:O	1:I:292[C]:LEU:CD1	2.68	0.40
1:I:406[C]:ILE:HG23	1:I:466[C]:ALA:HB2	2.04	0.40
1:J:59[C]:ASN:N	1:J:59[C]:ASN:ND2	2.68	0.40
1:J:122[C]:THR:OG1	1:J:128[C]:THR:HG22	2.22	0.40
1:J:448[C]:VAL:HG12	1:J:449[C]:CYS:N	2.35	0.40
2:L:166[C]:LEU:HD23	2:L:166[C]:LEU:HA	1.88	0.40
1:A:84[A]:ASN:ND2	1:A:84[A]:ASN:C	2.73	0.40
1:B:166[A]:VAL:HG22	1:B:274[A]:LEU:O	2.22	0.40
1:B:311[A]:LYS:O	1:B:313[A]:PRO:HD3	2.21	0.40
1:C:88[A]:MET:HE1	1:C:200[A]:LEU:HD21	2.04	0.40
1:C:467[A]:SER:OG	1:C:468[A]:PHE:N	2.55	0.40
1:H:71[A]:PHE:HD2	1:H:78[A]:MET:CE	2.35	0.40
1:I:289[A]:LEU:HD12	1:I:289[A]:LEU:N	2.33	0.40
3:I:4758[A]:FAD:HM83	3:I:4758[A]:FAD:HM71	1.84	0.40
2:K:132[A]:SER:O	2:K:135[A]:ALA:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:166[A]:LEU:HA	2:L:166[A]:LEU:HD23	1.84	0.40
2:M:152[A]:THR:O	2:M:157[A]:ILE:O	2.40	0.40
1:A:84[C]:ASN:ND2	1:A:84[C]:ASN:C	2.73	0.40
1:B:166[C]:VAL:HG22	1:B:274[C]:LEU:O	2.22	0.40
1:B:311[C]:LYS:O	1:B:313[C]:PRO:HD3	2.21	0.40
1:C:88[C]:MET:HE1	1:C:200[C]:LEU:HD21	2.04	0.40
1:C:467[C]:SER:OG	1:C:468[C]:PHE:N	2.55	0.40
1:H:71[C]:PHE:HD2	1:H:78[C]:MET:CE	2.35	0.40
3:H:4758[C]:FAD:HM83	3:H:4758[C]:FAD:HM71	1.84	0.40
1:I:289[C]:LEU:HD12	1:I:289[C]:LEU:N	2.33	0.40
2:K:158[C]:PHE:HZ	2:K:166[C]:LEU:HD23	1.85	0.40
1:A:74[A]:ARG:HH21	1:B:59[A]:ASN:ND2	2.18	0.40
1:A:452[A]:HIS:HA	1:A:453[A]:PRO:HA	1.76	0.40
1:B:149[A]:GLY:HA3	3:B:4751[A]:FAD:C5B	2.51	0.40
1:B:309[A]:GLN:HG2	1:B:316[A]:TYR:CE2	2.55	0.40
1:D:89[A]:MET:HE3	1:D:92[A]:LYS:CE	2.51	0.40
1:D:297[A]:ASP:CB	1:D:298[A]:PRO:HD2	2.47	0.40
1:E:85[A]:LEU:CD1	1:E:176[A]:LYS:HA	2.52	0.40
1:E:461[A]:GLU:OE1	1:E:472[A]:ILE:HG22	2.21	0.40
1:F:445[A]:ILE:HG21	1:F:463[A]:ASN:ND2	2.36	0.40
1:G:244[A]:THR:OG1	1:G:257[A]:SER:HB2	2.21	0.40
1:G:367[A]:VAL:HG22	1:G:436[A]:LEU:CD2	2.52	0.40
1:H:216[A]:VAL:C	1:H:218[A]:ILE:H	2.25	0.40
1:I:336[A]:ILE:HG22	1:I:337[A]:ILE:CG2	2.48	0.40
1:I:452[A]:HIS:HA	1:I:453[A]:PRO:HA	1.60	0.40
2:K:171[A]:GLN:C	2:K:173[A]:GLY:H	2.24	0.40
2:N:133[A]:PRO:O	2:N:136[A]:ARG:CG	2.69	0.40
1:A:74[C]:ARG:HH21	1:B:59[C]:ASN:ND2	2.18	0.40
1:A:452[C]:HIS:HA	1:A:453[C]:PRO:HA	1.76	0.40
3:A:4751[C]:FAD:C5B	1:B:149[C]:GLY:HA3	2.51	0.40
1:B:309[C]:GLN:HG2	1:B:316[C]:TYR:CE2	2.55	0.40
1:D:89[C]:MET:HE3	1:D:92[C]:LYS:CE	2.51	0.40
1:D:297[C]:ASP:CB	1:D:298[C]:PRO:HD2	2.47	0.40
1:E:85[C]:LEU:CD1	1:E:176[C]:LYS:HA	2.52	0.40
1:E:461[C]:GLU:OE1	1:E:472[C]:ILE:HG22	2.21	0.40
1:F:445[C]:ILE:HG21	1:F:463[C]:ASN:ND2	2.36	0.40
1:G:244[C]:THR:OG1	1:G:257[C]:SER:HB2	2.21	0.40
1:G:367[C]:VAL:HG22	1:G:436[C]:LEU:CD2	2.52	0.40
1:H:216[C]:VAL:C	1:H:218[C]:ILE:H	2.25	0.40
1:I:336[C]:ILE:HG22	1:I:337[C]:ILE:CG2	2.48	0.40
1:I:452[C]:HIS:HA	1:I:453[C]:PRO:HA	1.60	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:157[C]:ILE:H	2:M:157[C]:ILE:HG13	1.52	0.40
3:A:4750[A]:FAD:HM83	3:A:4750[A]:FAD:HM71	1.84	0.40
1:B:85[A]:LEU:O	1:B:86[A]:ASP:C	2.59	0.40
1:C:183[A]:VAL:O	1:C:206[A]:ALA:HA	2.22	0.40
1:D:15[A]:GLY:CA	1:D:43[A]:GLY:HA3	2.51	0.40
1:D:253[A]:LYS:HE2	1:D:272[A]:ASP:OD1	2.22	0.40
1:D:363[A]:GLU:HB2	1:D:425[A]:ALA:HB3	2.02	0.40
1:E:48[A]:VAL:HG23	1:E:48[A]:VAL:O	2.22	0.40
1:E:349[A]:ILE:HD13	1:E:351[A]:TYR:CZ	2.57	0.40
3:E:4754[A]:FAD:H9	3:E:4754[A]:FAD:H1'1	1.92	0.40
1:F:302[A]:ILE:HG13	1:F:321[A]:VAL:HG22	2.03	0.40
1:F:351[A]:TYR:O	1:F:354[A]:VAL:HG12	2.22	0.40
1:G:305[A]:ASN:HD21	1:G:309[A]:GLN:HE21	1.70	0.40
1:H:50[A]:CYS:SG	3:H:4757[A]:FAD:C4X	3.09	0.40
1:H:155[A]:PHE:CB	1:H:278[A]:ILE:HD11	2.52	0.40
1:I:446[A]:ALA:HB1	1:I:464[A]:LEU:HD12	2.03	0.40
1:J:299[A]:ARG:HH11	1:J:301[A]:ARG:NH2	2.19	0.40
2:L:158[A]:PHE:CZ	2:L:166[A]:LEU:HD12	2.56	0.40
1:B:85[C]:LEU:O	1:B:86[C]:ASP:C	2.59	0.40
1:C:183[C]:VAL:O	1:C:206[C]:ALA:HA	2.22	0.40
1:D:15[C]:GLY:CA	1:D:43[C]:GLY:HA3	2.51	0.40
1:D:253[C]:LYS:HE2	1:D:272[C]:ASP:OD1	2.22	0.40
1:D:363[C]:GLU:HB2	1:D:425[C]:ALA:HB3	2.02	0.40
3:D:4754[C]:FAD:H9	3:D:4754[C]:FAD:H1'1	1.92	0.40
1:E:48[C]:VAL:HG23	1:E:48[C]:VAL:O	2.22	0.40
1:E:349[C]:ILE:HD13	1:E:351[C]:TYR:CZ	2.57	0.40
1:F:302[C]:ILE:HG13	1:F:321[C]:VAL:HG22	2.03	0.40
1:F:351[C]:TYR:O	1:F:354[C]:VAL:HG12	2.22	0.40
1:G:305[C]:ASN:HD21	1:G:309[C]:GLN:HE21	1.70	0.40
3:G:4757[C]:FAD:C4X	1:H:50[C]:CYS:SG	3.09	0.40
1:H:155[C]:PHE:CB	1:H:278[C]:ILE:HD11	2.52	0.40
1:I:446[C]:ALA:HB1	1:I:464[C]:LEU:HD12	2.03	0.40
1:J:299[C]:ARG:HH11	1:J:301[C]:ARG:NH2	2.19	0.40
2:L:142[C]:HIS:O	2:L:143[C]:SER:C	2.59	0.40
3:O:4750[C]:FAD:HM83	3:O:4750[C]:FAD:HM71	1.84	0.40

There are no symmetry-related clashes.

## 4.3 Torsion angles [i](#)

### 4.3.1 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	1-A	473/474 (100%)	426 (90%)	40 (8%)	7 (2%)	10	21
1	1-B	473/474 (100%)	418 (88%)	47 (10%)	8 (2%)	9	18
1	1-C	473/474 (100%)	434 (92%)	32 (7%)	7 (2%)	10	21
1	1-D	473/474 (100%)	418 (88%)	41 (9%)	14 (3%)	4	7
1	1-E	473/474 (100%)	436 (92%)	33 (7%)	4 (1%)	19	39
1	1-F	473/474 (100%)	425 (90%)	43 (9%)	5 (1%)	14	30
1	1-G	473/474 (100%)	425 (90%)	40 (8%)	8 (2%)	9	18
1	1-H	473/474 (100%)	431 (91%)	33 (7%)	9 (2%)	8	15
1	1-I	473/474 (100%)	406 (86%)	51 (11%)	16 (3%)	3	5
1	1-J	473/474 (100%)	399 (84%)	57 (12%)	17 (4%)	3	4
1	2-A	473/474 (100%)	426 (90%)	40 (8%)	7 (2%)	10	21
1	2-B	473/474 (100%)	418 (88%)	47 (10%)	8 (2%)	9	18
1	2-C	473/474 (100%)	434 (92%)	32 (7%)	7 (2%)	10	21
1	2-D	473/474 (100%)	418 (88%)	41 (9%)	14 (3%)	4	7
1	2-E	473/474 (100%)	436 (92%)	33 (7%)	4 (1%)	19	39
1	2-F	473/474 (100%)	425 (90%)	43 (9%)	5 (1%)	14	30
1	2-G	473/474 (100%)	425 (90%)	40 (8%)	8 (2%)	9	18
1	2-H	473/474 (100%)	431 (91%)	33 (7%)	9 (2%)	8	15
1	2-I	473/474 (100%)	406 (86%)	51 (11%)	16 (3%)	3	5
1	2-J	473/474 (100%)	399 (84%)	57 (12%)	17 (4%)	3	4
2	1-K	42/229 (18%)	28 (67%)	9 (21%)	5 (12%)	0	0
2	1-L	42/229 (18%)	28 (67%)	6 (14%)	8 (19%)	0	0
2	1-M	42/229 (18%)	31 (74%)	8 (19%)	3 (7%)	1	1
2	1-N	42/229 (18%)	33 (79%)	7 (17%)	2 (5%)	2	2
2	1-O	42/229 (18%)	31 (74%)	8 (19%)	3 (7%)	1	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	2-K	40/229 (18%)	31 (78%)	6 (15%)	3 (8%)	1	1
2	2-L	40/229 (18%)	26 (65%)	10 (25%)	4 (10%)	0	0
2	2-M	41/229 (18%)	30 (73%)	8 (20%)	3 (7%)	1	1
2	2-N	40/229 (18%)	26 (65%)	7 (18%)	7 (18%)	0	0
All	All	9831/11541 (85%)	8700 (88%)	903 (9%)	228 (2%)	6	11

All (228) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1-A	263[A]	GLY
1	1-B	2[A]	ASP
1	1-B	79[A]	SER
1	1-B	262[A]	SER
1	1-B	413[A]	ASP
1	1-C	2[A]	ASP
1	1-C	79[A]	SER
1	1-D	132[A]	ALA
1	1-D	263[A]	GLY
1	1-E	263[A]	GLY
1	1-F	79[A]	SER
1	1-F	124[A]	LYS
1	1-G	50[A]	CYS
1	1-G	50[B]	CYS
1	1-G	344[A]	GLY
1	1-H	263[A]	GLY
1	1-I	124[A]	LYS
1	1-I	266[A]	ALA
1	1-I	267[A]	GLU
1	1-I	373[A]	GLN
1	1-I	397[A]	ASN
1	1-J	136[A]	THR
1	1-J	440[A]	ALA
2	1-K	154[A]	PRO
2	1-K	172[A]	THR
2	1-L	140[A]	GLU
2	1-L	143[A]	SER
1	2-A	263[C]	GLY
1	2-B	2[C]	ASP
1	2-B	79[C]	SER
1	2-B	262[C]	SER
1	2-B	413[C]	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	2-C	2[C]	ASP
1	2-C	79[C]	SER
1	2-D	132[C]	ALA
1	2-D	263[C]	GLY
1	2-E	263[C]	GLY
1	2-F	79[C]	SER
1	2-F	124[C]	LYS
1	2-G	50[C]	CYS
1	2-G	50[D]	CYS
1	2-G	344[C]	GLY
1	2-H	263[C]	GLY
1	2-I	124[C]	LYS
1	2-I	266[C]	ALA
1	2-I	267[C]	GLU
1	2-I	373[C]	GLN
1	2-I	397[C]	ASN
1	2-J	136[C]	THR
1	2-J	440[C]	ALA
2	2-K	154[C]	PRO
2	2-L	148[C]	GLN
2	2-L	154[C]	PRO
2	2-M	154[C]	PRO
2	2-N	138[C]	ILE
2	2-N	149[C]	GLY
2	2-N	154[C]	PRO
2	2-N	156[C]	GLY
1	1-A	2[A]	ASP
1	1-A	50[A]	CYS
1	1-A	50[B]	CYS
1	1-A	429[A]	VAL
1	1-B	134[A]	GLY
1	1-B	291[A]	GLU
1	1-C	215[A]	GLY
1	1-C	263[A]	GLY
1	1-D	215[A]	GLY
1	1-E	202[A]	ALA
1	1-H	259[A]	GLU
1	1-H	262[A]	SER
1	1-I	263[A]	GLY
1	1-I	377[A]	GLU
1	1-I	469[A]	GLY
1	1-J	132[A]	ALA

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	1-J	253[A]	LYS
1	1-J	310[A]	THR
2	1-K	153[A]	GLY
2	1-L	167[A]	VAL
2	1-N	143[A]	SER
2	1-O	139[A]	LEU
1	2-A	2[C]	ASP
1	2-A	50[C]	CYS
1	2-A	50[D]	CYS
1	2-A	429[C]	VAL
1	2-B	134[C]	GLY
1	2-B	291[C]	GLU
1	2-C	215[C]	GLY
1	2-C	263[C]	GLY
1	2-D	215[C]	GLY
1	2-E	202[C]	ALA
1	2-H	259[C]	GLU
1	2-H	262[C]	SER
1	2-I	263[C]	GLY
1	2-I	377[C]	GLU
1	2-I	469[C]	GLY
1	2-J	132[C]	ALA
1	2-J	253[C]	LYS
1	2-J	310[C]	THR
2	2-K	143[C]	SER
2	2-M	143[C]	SER
2	2-M	155[C]	ARG
2	2-N	148[C]	GLN
2	2-N	169[C]	LEU
1	1-A	79[A]	SER
1	1-C	124[A]	LYS
1	1-D	136[A]	THR
1	1-D	360[A]	THR
1	1-D	468[A]	PHE
1	1-G	266[A]	ALA
1	1-I	285[A]	LYS
1	1-J	79[A]	SER
1	1-J	109[A]	GLN
1	1-J	110[A]	ASN
1	1-J	120[A]	LYS
1	1-J	467[A]	SER
2	1-L	154[A]	PRO

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	1-L	166[A]	LEU
2	1-M	133[A]	PRO
2	1-M	150[A]	THR
2	1-N	147[A]	SER
1	2-A	79[C]	SER
1	2-C	124[C]	LYS
1	2-D	136[C]	THR
1	2-D	360[C]	THR
1	2-D	468[C]	PHE
1	2-G	266[C]	ALA
1	2-I	285[C]	LYS
1	2-J	79[C]	SER
1	2-J	109[C]	GLN
1	2-J	110[C]	ASN
1	2-J	120[C]	LYS
1	2-J	467[C]	SER
2	2-L	169[C]	LEU
1	1-C	174[A]	LEU
1	1-D	131[A]	LYS
1	1-D	456[A]	SER
1	1-F	48[A]	VAL
1	1-G	259[A]	GLU
1	1-H	70[A]	ASP
1	1-H	79[A]	SER
1	1-I	262[A]	SER
1	1-I	313[A]	PRO
1	1-I	372[A]	GLU
2	1-K	148[A]	GLN
2	1-L	133[A]	PRO
2	1-O	154[A]	PRO
1	2-C	174[C]	LEU
1	2-D	131[C]	LYS
1	2-D	456[C]	SER
1	2-F	48[C]	VAL
1	2-G	259[C]	GLU
1	2-H	70[C]	ASP
1	2-H	79[C]	SER
1	2-I	262[C]	SER
1	2-I	313[C]	PRO
1	2-I	372[C]	GLU
1	1-B	50[A]	CYS
1	1-B	50[B]	CYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	1-D	3[A]	GLN
1	1-D	45[A]	CYS
1	1-D	262[A]	SER
1	1-G	134[A]	GLY
1	1-G	263[A]	GLY
1	1-H	215[A]	GLY
1	1-H	345[A]	GLY
1	1-I	48[A]	VAL
1	1-I	297[A]	ASP
1	1-J	130[A]	THR
1	1-J	131[A]	LYS
1	1-J	162[A]	GLU
2	1-K	171[A]	GLN
2	1-L	139[A]	LEU
2	1-M	154[A]	PRO
1	2-B	50[C]	CYS
1	2-B	50[D]	CYS
1	2-D	3[C]	GLN
1	2-D	45[C]	CYS
1	2-D	262[C]	SER
1	2-G	134[C]	GLY
1	2-G	263[C]	GLY
1	2-H	215[C]	GLY
1	2-H	345[C]	GLY
1	2-I	48[C]	VAL
1	2-I	297[C]	ASP
1	2-J	130[C]	THR
1	2-J	131[C]	LYS
1	2-J	162[C]	GLU
2	2-L	165[C]	LYS
2	2-N	170[C]	LYS
1	1-A	433[A]	ALA
1	1-C	48[A]	VAL
1	1-D	134[A]	GLY
1	1-D	347[A]	VAL
1	1-F	263[A]	GLY
1	1-H	48[A]	VAL
1	1-H	91[A]	GLN
1	1-I	360[A]	THR
1	1-J	347[A]	VAL
2	1-L	155[A]	ARG
1	2-A	433[C]	ALA

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Mol	Chain	Res	Type
1	2-C	48[C]	VAL
1	2-D	134[C]	GLY
1	2-D	347[C]	VAL
1	2-F	263[C]	GLY
1	2-H	48[C]	VAL
1	2-H	91[C]	GLN
1	2-I	360[C]	THR
1	2-J	347[C]	VAL
1	1-E	4[A]	PRO
1	1-G	135[A]	GLY
1	1-J	263[A]	GLY
2	1-O	156[A]	GLY
1	2-E	4[C]	PRO
1	2-G	135[C]	GLY
1	2-J	263[C]	GLY
1	1-I	4[A]	PRO
1	2-I	4[C]	PRO
2	2-K	133[C]	PRO
1	1-D	297[A]	ASP
1	1-J	215[A]	GLY
1	2-D	297[C]	ASP
1	2-J	215[C]	GLY
1	1-E	48[A]	VAL
1	1-F	345[A]	GLY
1	2-E	48[C]	VAL
1	2-F	345[C]	GLY
1	1-J	156[A]	PRO
1	2-J	156[C]	PRO

#### 4.3.2 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	1-A	374/373 (100%)	308 (82%)	66 (18%)	2 3
1	1-B	374/373 (100%)	307 (82%)	67 (18%)	2 2
1	1-C	374/373 (100%)	317 (85%)	57 (15%)	3 4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1-D	374/373 (100%)	304 (81%)	70 (19%)	1	2
1	1-E	374/373 (100%)	311 (83%)	63 (17%)	2	3
1	1-F	374/373 (100%)	311 (83%)	63 (17%)	2	3
1	1-G	374/373 (100%)	310 (83%)	64 (17%)	2	3
1	1-H	374/373 (100%)	311 (83%)	63 (17%)	2	3
1	1-I	374/373 (100%)	316 (84%)	58 (16%)	2	4
1	1-J	374/373 (100%)	295 (79%)	79 (21%)	1	2
2	1-K	35/195 (18%)	29 (83%)	6 (17%)	2	3
2	1-L	35/195 (18%)	23 (66%)	12 (34%)	0	0
2	1-M	35/195 (18%)	26 (74%)	9 (26%)	0	1
2	1-N	35/195 (18%)	30 (86%)	5 (14%)	3	5
2	1-O	35/195 (18%)	28 (80%)	7 (20%)	1	2
All	All	3915/4705 (83%)	3226 (82%)	689 (18%)	2	3

All (689) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1-A	3[A]	GLN
1	1-A	19[A]	TYR
1	1-A	24[A]	LYS
1	1-A	31[A]	LYS
1	1-A	33[A]	VAL
1	1-A	37[A]	LYS
1	1-A	44[A]	THR
1	1-A	46[A]	LEU
1	1-A	54[A]	LYS
1	1-A	56[A]	LEU
1	1-A	73[A]	SER
1	1-A	78[A]	MET
1	1-A	79[A]	SER
1	1-A	80[A]	GLU
1	1-A	82[A]	ARG
1	1-A	84[A]	ASN
1	1-A	85[A]	LEU
1	1-A	92[A]	LYS
1	1-A	93[A]	SER
1	1-A	97[A]	LYS
1	1-A	99[A]	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	1-A	118[A]	TYR
1	1-A	136[A]	THR
1	1-A	137[A]	GLN
1	1-A	142[A]	LYS
1	1-A	159[A]	THR
1	1-A	162[A]	GLU
1	1-A	174[A]	LEU
1	1-A	180[A]	LYS
1	1-A	200[A]	LEU
1	1-A	203[A]	ASP
1	1-A	207[A]	VAL
1	1-A	216[A]	VAL
1	1-A	230[A]	LEU
1	1-A	235[A]	PHE
1	1-A	236[A]	LYS
1	1-A	238[A]	LYS
1	1-A	242[A]	LYS
1	1-A	243[A]	VAL
1	1-A	248[A]	LYS
1	1-A	250[A]	SER
1	1-A	262[A]	SER
1	1-A	278[A]	ILE
1	1-A	281[A]	ARG
1	1-A	284[A]	THR
1	1-A	287[A]	LEU
1	1-A	290[A]	GLU
1	1-A	291[A]	GLU
1	1-A	297[A]	ASP
1	1-A	316[A]	TYR
1	1-A	320[A]	ASP
1	1-A	333[A]	ASP
1	1-A	336[A]	ILE
1	1-A	337[A]	ILE
1	1-A	349[A]	ILE
1	1-A	358[A]	ILE
1	1-A	383[A]	VAL
1	1-A	397[A]	ASN
1	1-A	409[A]	GLN
1	1-A	429[A]	VAL
1	1-A	437[A]	GLU
1	1-A	443[A]	GLU
1	1-A	445[A]	ILE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	1-A	447[A]	ARG
1	1-A	456[A]	SER
1	1-A	457[A]	GLU
1	1-B	6[A]	ASP
1	1-B	9[A]	VAL
1	1-B	19[A]	TYR
1	1-B	27[A]	GLN
1	1-B	28[A]	LEU
1	1-B	32[A]	THR
1	1-B	39[A]	GLU
1	1-B	54[A]	LYS
1	1-B	69[A]	LYS
1	1-B	77[A]	GLU
1	1-B	79[A]	SER
1	1-B	83[A]	LEU
1	1-B	86[A]	ASP
1	1-B	91[A]	GLN
1	1-B	108[A]	LYS
1	1-B	118[A]	TYR
1	1-B	124[A]	LYS
1	1-B	137[A]	GLN
1	1-B	141[A]	THR
1	1-B	142[A]	LYS
1	1-B	144[A]	ILE
1	1-B	163[A]	ASP
1	1-B	164[A]	THR
1	1-B	172[A]	LEU
1	1-B	174[A]	LEU
1	1-B	180[A]	LYS
1	1-B	200[A]	LEU
1	1-B	218[A]	ILE
1	1-B	220[A]	MET
1	1-B	221[A]	GLU
1	1-B	222[A]	ILE
1	1-B	224[A]	LYS
1	1-B	228[A]	ARG
1	1-B	240[A]	ASN
1	1-B	243[A]	VAL
1	1-B	247[A]	THR
1	1-B	248[A]	LYS
1	1-B	249[A]	LYS
1	1-B	250[A]	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	1-B	253[A]	LYS
1	1-B	255[A]	ASP
1	1-B	262[A]	SER
1	1-B	272[A]	ASP
1	1-B	275[A]	LEU
1	1-B	280[A]	ARG
1	1-B	281[A]	ARG
1	1-B	289[A]	LEU
1	1-B	297[A]	ASP
1	1-B	305[A]	ASN
1	1-B	307[A]	ARG
1	1-B	318[A]	ILE
1	1-B	337[A]	ILE
1	1-B	354[A]	VAL
1	1-B	369[A]	LYS
1	1-B	372[A]	GLU
1	1-B	374[A]	LEU
1	1-B	380[A]	GLU
1	1-B	383[A]	VAL
1	1-B	400[A]	THR
1	1-B	403[A]	MET
1	1-B	406[A]	ILE
1	1-B	409[A]	GLN
1	1-B	414[A]	ARG
1	1-B	447[A]	ARG
1	1-B	455[A]	LEU
1	1-B	468[A]	PHE
1	1-B	470[A]	LYS
1	1-C	3[A]	GLN
1	1-C	19[A]	TYR
1	1-C	32[A]	THR
1	1-C	33[A]	VAL
1	1-C	40[A]	THR
1	1-C	44[A]	THR
1	1-C	53[A]	SER
1	1-C	54[A]	LYS
1	1-C	69[A]	LYS
1	1-C	80[A]	GLU
1	1-C	85[A]	LEU
1	1-C	86[A]	ASP
1	1-C	87[A]	LYS
1	1-C	89[A]	MET

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	1-C	97[A]	LYS
1	1-C	99[A]	LEU
1	1-C	111[A]	LYS
1	1-C	118[A]	TYR
1	1-C	120[A]	LYS
1	1-C	131[A]	LYS
1	1-C	137[A]	GLN
1	1-C	139[A]	ILE
1	1-C	145[A]	LEU
1	1-C	162[A]	GLU
1	1-C	169[A]	THR
1	1-C	174[A]	LEU
1	1-C	180[A]	LYS
1	1-C	182[A]	VAL
1	1-C	200[A]	LEU
1	1-C	203[A]	ASP
1	1-C	210[A]	LEU
1	1-C	222[A]	ILE
1	1-C	224[A]	LYS
1	1-C	230[A]	LEU
1	1-C	235[A]	PHE
1	1-C	239[A]	LEU
1	1-C	242[A]	LYS
1	1-C	247[A]	THR
1	1-C	249[A]	LYS
1	1-C	255[A]	ASP
1	1-C	258[A]	ILE
1	1-C	269[A]	ILE
1	1-C	275[A]	LEU
1	1-C	281[A]	ARG
1	1-C	290[A]	GLU
1	1-C	297[A]	ASP
1	1-C	306[A]	THR
1	1-C	311[A]	LYS
1	1-C	322[A]	VAL
1	1-C	330[A]	LYS
1	1-C	333[A]	ASP
1	1-C	358[A]	ILE
1	1-C	414[A]	ARG
1	1-C	437[A]	GLU
1	1-C	445[A]	ILE
1	1-C	447[A]	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	1-C	455[A]	LEU
1	1-D	6[A]	ASP
1	1-D	8[A]	ASP
1	1-D	19[A]	TYR
1	1-D	28[A]	LEU
1	1-D	32[A]	THR
1	1-D	39[A]	GLU
1	1-D	50[A]	CYS
1	1-D	50[B]	CYS
1	1-D	54[A]	LYS
1	1-D	69[A]	LYS
1	1-D	77[A]	GLU
1	1-D	78[A]	MET
1	1-D	82[A]	ARG
1	1-D	83[A]	LEU
1	1-D	87[A]	LYS
1	1-D	91[A]	GLN
1	1-D	97[A]	LYS
1	1-D	108[A]	LYS
1	1-D	111[A]	LYS
1	1-D	120[A]	LYS
1	1-D	121[A]	ILE
1	1-D	130[A]	THR
1	1-D	133[A]	ASP
1	1-D	144[A]	ILE
1	1-D	145[A]	LEU
1	1-D	151[A]	GLU
1	1-D	159[A]	THR
1	1-D	162[A]	GLU
1	1-D	165[A]	ILE
1	1-D	166[A]	VAL
1	1-D	169[A]	THR
1	1-D	172[A]	LEU
1	1-D	188[A]	VAL
1	1-D	191[A]	VAL
1	1-D	195[A]	SER
1	1-D	200[A]	LEU
1	1-D	209[A]	PHE
1	1-D	218[A]	ILE
1	1-D	224[A]	LYS
1	1-D	235[A]	PHE
1	1-D	249[A]	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	1-D	253[A]	LYS
1	1-D	255[A]	ASP
1	1-D	270[A]	THR
1	1-D	272[A]	ASP
1	1-D	275[A]	LEU
1	1-D	281[A]	ARG
1	1-D	292[A]	LEU
1	1-D	296[A]	LEU
1	1-D	301[A]	ARG
1	1-D	305[A]	ASN
1	1-D	316[A]	TYR
1	1-D	318[A]	ILE
1	1-D	321[A]	VAL
1	1-D	333[A]	ASP
1	1-D	354[A]	VAL
1	1-D	356[A]	SER
1	1-D	372[A]	GLU
1	1-D	374[A]	LEU
1	1-D	376[A]	GLU
1	1-D	382[A]	LYS
1	1-D	383[A]	VAL
1	1-D	385[A]	LYS
1	1-D	393[A]	ARG
1	1-D	403[A]	MET
1	1-D	410[A]	LYS
1	1-D	414[A]	ARG
1	1-D	416[A]	LEU
1	1-D	427[A]	GLU
1	1-D	470[A]	LYS
1	1-E	6[A]	ASP
1	1-E	19[A]	TYR
1	1-E	20[A]	VAL
1	1-E	33[A]	VAL
1	1-E	39[A]	GLU
1	1-E	54[A]	LYS
1	1-E	56[A]	LEU
1	1-E	69[A]	LYS
1	1-E	74[A]	ARG
1	1-E	78[A]	MET
1	1-E	79[A]	SER
1	1-E	84[A]	ASN
1	1-E	85[A]	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	1-E	86[A]	ASP
1	1-E	90[A]	GLU
1	1-E	94[A]	THR
1	1-E	97[A]	LYS
1	1-E	99[A]	LEU
1	1-E	109[A]	GLN
1	1-E	116[A]	ASN
1	1-E	131[A]	LYS
1	1-E	137[A]	GLN
1	1-E	145[A]	LEU
1	1-E	162[A]	GLU
1	1-E	164[A]	THR
1	1-E	169[A]	THR
1	1-E	176[A]	LYS
1	1-E	177[A]	VAL
1	1-E	179[A]	GLU
1	1-E	180[A]	LYS
1	1-E	200[A]	LEU
1	1-E	222[A]	ILE
1	1-E	224[A]	LYS
1	1-E	228[A]	ARG
1	1-E	230[A]	LEU
1	1-E	235[A]	PHE
1	1-E	236[A]	LYS
1	1-E	243[A]	VAL
1	1-E	247[A]	THR
1	1-E	254[A]	ILE
1	1-E	255[A]	ASP
1	1-E	270[A]	THR
1	1-E	275[A]	LEU
1	1-E	278[A]	ILE
1	1-E	281[A]	ARG
1	1-E	291[A]	GLU
1	1-E	305[A]	ASN
1	1-E	306[A]	THR
1	1-E	311[A]	LYS
1	1-E	312[A]	ILE
1	1-E	336[A]	ILE
1	1-E	349[A]	ILE
1	1-E	354[A]	VAL
1	1-E	382[A]	LYS
1	1-E	383[A]	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	1-E	392[A]	SER
1	1-E	412[A]	THR
1	1-E	420[A]	ILE
1	1-E	427[A]	GLU
1	1-E	436[A]	LEU
1	1-E	447[A]	ARG
1	1-E	455[A]	LEU
1	1-E	472[A]	ILE
1	1-F	5[A]	ILE
1	1-F	12[A]	ILE
1	1-F	19[A]	TYR
1	1-F	32[A]	THR
1	1-F	33[A]	VAL
1	1-F	44[A]	THR
1	1-F	54[A]	LYS
1	1-F	69[A]	LYS
1	1-F	71[A]	PHE
1	1-F	84[A]	ASN
1	1-F	91[A]	GLN
1	1-F	94[A]	THR
1	1-F	114[A]	HIS
1	1-F	116[A]	ASN
1	1-F	120[A]	LYS
1	1-F	130[A]	THR
1	1-F	144[A]	ILE
1	1-F	151[A]	GLU
1	1-F	158[A]	ILE
1	1-F	159[A]	THR
1	1-F	162[A]	GLU
1	1-F	164[A]	THR
1	1-F	169[A]	THR
1	1-F	172[A]	LEU
1	1-F	175[A]	LYS
1	1-F	176[A]	LYS
1	1-F	179[A]	GLU
1	1-F	188[A]	VAL
1	1-F	210[A]	LEU
1	1-F	218[A]	ILE
1	1-F	224[A]	LYS
1	1-F	235[A]	PHE
1	1-F	243[A]	VAL
1	1-F	253[A]	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	1-F	255[A]	ASP
1	1-F	257[A]	SER
1	1-F	270[A]	THR
1	1-F	275[A]	LEU
1	1-F	280[A]	ARG
1	1-F	281[A]	ARG
1	1-F	284[A]	THR
1	1-F	289[A]	LEU
1	1-F	290[A]	GLU
1	1-F	291[A]	GLU
1	1-F	295[A]	GLU
1	1-F	301[A]	ARG
1	1-F	309[A]	GLN
1	1-F	312[A]	ILE
1	1-F	315[A]	ILE
1	1-F	318[A]	ILE
1	1-F	330[A]	LYS
1	1-F	339[A]	VAL
1	1-F	372[A]	GLU
1	1-F	374[A]	LEU
1	1-F	376[A]	GLU
1	1-F	380[A]	GLU
1	1-F	383[A]	VAL
1	1-F	406[A]	ILE
1	1-F	409[A]	GLN
1	1-F	414[A]	ARG
1	1-F	447[A]	ARG
1	1-F	455[A]	LEU
1	1-F	470[A]	LYS
1	1-G	2[A]	ASP
1	1-G	19[A]	TYR
1	1-G	32[A]	THR
1	1-G	40[A]	THR
1	1-G	44[A]	THR
1	1-G	46[A]	LEU
1	1-G	54[A]	LYS
1	1-G	56[A]	LEU
1	1-G	69[A]	LYS
1	1-G	78[A]	MET
1	1-G	79[A]	SER
1	1-G	82[A]	ARG
1	1-G	84[A]	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	1-G	90[A]	GLU
1	1-G	91[A]	GLN
1	1-G	107[A]	PHE
1	1-G	111[A]	LYS
1	1-G	126[A]	GLN
1	1-G	131[A]	LYS
1	1-G	136[A]	THR
1	1-G	141[A]	THR
1	1-G	145[A]	LEU
1	1-G	151[A]	GLU
1	1-G	162[A]	GLU
1	1-G	165[A]	ILE
1	1-G	189[A]	ILE
1	1-G	191[A]	VAL
1	1-G	200[A]	LEU
1	1-G	210[A]	LEU
1	1-G	222[A]	ILE
1	1-G	230[A]	LEU
1	1-G	235[A]	PHE
1	1-G	239[A]	LEU
1	1-G	242[A]	LYS
1	1-G	248[A]	LYS
1	1-G	254[A]	ILE
1	1-G	255[A]	ASP
1	1-G	258[A]	ILE
1	1-G	265[A]	LYS
1	1-G	274[A]	LEU
1	1-G	275[A]	LEU
1	1-G	281[A]	ARG
1	1-G	284[A]	THR
1	1-G	289[A]	LEU
1	1-G	292[A]	LEU
1	1-G	297[A]	ASP
1	1-G	299[A]	ARG
1	1-G	304[A]	VAL
1	1-G	307[A]	ARG
1	1-G	309[A]	GLN
1	1-G	314[A]	ASN
1	1-G	322[A]	VAL
1	1-G	330[A]	LYS
1	1-G	349[A]	ILE
1	1-G	354[A]	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	1-G	358[A]	ILE
1	1-G	383[A]	VAL
1	1-G	403[A]	MET
1	1-G	420[A]	ILE
1	1-G	421[A]	LEU
1	1-G	436[A]	LEU
1	1-G	445[A]	ILE
1	1-G	455[A]	LEU
1	1-G	472[A]	ILE
1	1-H	5[A]	ILE
1	1-H	19[A]	TYR
1	1-H	32[A]	THR
1	1-H	41[A]	LEU
1	1-H	44[A]	THR
1	1-H	54[A]	LYS
1	1-H	79[A]	SER
1	1-H	82[A]	ARG
1	1-H	83[A]	LEU
1	1-H	87[A]	LYS
1	1-H	91[A]	GLN
1	1-H	114[A]	HIS
1	1-H	124[A]	LYS
1	1-H	142[A]	LYS
1	1-H	144[A]	ILE
1	1-H	164[A]	THR
1	1-H	168[A]	SER
1	1-H	169[A]	THR
1	1-H	172[A]	LEU
1	1-H	174[A]	LEU
1	1-H	176[A]	LYS
1	1-H	191[A]	VAL
1	1-H	193[A]	LEU
1	1-H	195[A]	SER
1	1-H	200[A]	LEU
1	1-H	216[A]	VAL
1	1-H	235[A]	PHE
1	1-H	241[A]	THR
1	1-H	242[A]	LYS
1	1-H	243[A]	VAL
1	1-H	250[A]	SER
1	1-H	254[A]	ILE
1	1-H	255[A]	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	1-H	257[A]	SER
1	1-H	262[A]	SER
1	1-H	265[A]	LYS
1	1-H	269[A]	ILE
1	1-H	270[A]	THR
1	1-H	272[A]	ASP
1	1-H	285[A]	LYS
1	1-H	292[A]	LEU
1	1-H	305[A]	ASN
1	1-H	307[A]	ARG
1	1-H	330[A]	LYS
1	1-H	347[A]	VAL
1	1-H	360[A]	THR
1	1-H	363[A]	GLU
1	1-H	372[A]	GLU
1	1-H	374[A]	LEU
1	1-H	376[A]	GLU
1	1-H	397[A]	ASN
1	1-H	400[A]	THR
1	1-H	403[A]	MET
1	1-H	406[A]	ILE
1	1-H	409[A]	GLN
1	1-H	414[A]	ARG
1	1-H	415[A]	VAL
1	1-H	447[A]	ARG
1	1-H	454[A]	THR
1	1-H	455[A]	LEU
1	1-H	456[A]	SER
1	1-H	460[A]	ARG
1	1-H	470[A]	LYS
1	1-I	6[A]	ASP
1	1-I	8[A]	ASP
1	1-I	11[A]	VAL
1	1-I	24[A]	LYS
1	1-I	27[A]	GLN
1	1-I	32[A]	THR
1	1-I	33[A]	VAL
1	1-I	37[A]	LYS
1	1-I	38[A]	ASN
1	1-I	41[A]	LEU
1	1-I	54[A]	LYS
1	1-I	56[A]	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	1-I	76[A]	ILE
1	1-I	85[A]	LEU
1	1-I	110[A]	ASN
1	1-I	115[A]	VAL
1	1-I	118[A]	TYR
1	1-I	121[A]	ILE
1	1-I	140[A]	ASP
1	1-I	141[A]	THR
1	1-I	142[A]	LYS
1	1-I	162[A]	GLU
1	1-I	164[A]	THR
1	1-I	169[A]	THR
1	1-I	177[A]	VAL
1	1-I	180[A]	LYS
1	1-I	182[A]	VAL
1	1-I	193[A]	LEU
1	1-I	195[A]	SER
1	1-I	208[A]	GLU
1	1-I	216[A]	VAL
1	1-I	218[A]	ILE
1	1-I	224[A]	LYS
1	1-I	230[A]	LEU
1	1-I	235[A]	PHE
1	1-I	236[A]	LYS
1	1-I	247[A]	THR
1	1-I	249[A]	LYS
1	1-I	256[A]	VAL
1	1-I	272[A]	ASP
1	1-I	275[A]	LEU
1	1-I	278[A]	ILE
1	1-I	284[A]	THR
1	1-I	289[A]	LEU
1	1-I	295[A]	GLU
1	1-I	297[A]	ASP
1	1-I	299[A]	ARG
1	1-I	333[A]	ASP
1	1-I	336[A]	ILE
1	1-I	337[A]	ILE
1	1-I	358[A]	ILE
1	1-I	381[A]	TYR
1	1-I	392[A]	SER
1	1-I	403[A]	MET

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	1-I	414[A]	ARG
1	1-I	447[A]	ARG
1	1-I	455[A]	LEU
1	1-I	471[A]	SER
1	1-J	12[A]	ILE
1	1-J	28[A]	LEU
1	1-J	35[A]	ILE
1	1-J	40[A]	THR
1	1-J	44[A]	THR
1	1-J	54[A]	LYS
1	1-J	69[A]	LYS
1	1-J	78[A]	MET
1	1-J	82[A]	ARG
1	1-J	83[A]	LEU
1	1-J	86[A]	ASP
1	1-J	91[A]	GLN
1	1-J	92[A]	LYS
1	1-J	97[A]	LYS
1	1-J	111[A]	LYS
1	1-J	113[A]	VAL
1	1-J	118[A]	TYR
1	1-J	121[A]	ILE
1	1-J	122[A]	THR
1	1-J	124[A]	LYS
1	1-J	128[A]	THR
1	1-J	133[A]	ASP
1	1-J	136[A]	THR
1	1-J	144[A]	ILE
1	1-J	158[A]	ILE
1	1-J	164[A]	THR
1	1-J	169[A]	THR
1	1-J	172[A]	LEU
1	1-J	174[A]	LEU
1	1-J	176[A]	LYS
1	1-J	180[A]	LYS
1	1-J	200[A]	LEU
1	1-J	204[A]	VAL
1	1-J	209[A]	PHE
1	1-J	216[A]	VAL
1	1-J	228[A]	ARG
1	1-J	232[A]	LYS
1	1-J	235[A]	PHE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	1-J	236[A]	LYS
1	1-J	238[A]	LYS
1	1-J	243[A]	VAL
1	1-J	247[A]	THR
1	1-J	265[A]	LYS
1	1-J	270[A]	THR
1	1-J	275[A]	LEU
1	1-J	278[A]	ILE
1	1-J	280[A]	ARG
1	1-J	281[A]	ARG
1	1-J	284[A]	THR
1	1-J	285[A]	LYS
1	1-J	290[A]	GLU
1	1-J	291[A]	GLU
1	1-J	294[A]	ILE
1	1-J	297[A]	ASP
1	1-J	299[A]	ARG
1	1-J	305[A]	ASN
1	1-J	307[A]	ARG
1	1-J	311[A]	LYS
1	1-J	315[A]	ILE
1	1-J	316[A]	TYR
1	1-J	321[A]	VAL
1	1-J	333[A]	ASP
1	1-J	336[A]	ILE
1	1-J	337[A]	ILE
1	1-J	354[A]	VAL
1	1-J	360[A]	THR
1	1-J	369[A]	LYS
1	1-J	372[A]	GLU
1	1-J	374[A]	LEU
1	1-J	393[A]	ARG
1	1-J	396[A]	THR
1	1-J	406[A]	ILE
1	1-J	413[A]	ASP
1	1-J	421[A]	LEU
1	1-J	436[A]	LEU
1	1-J	443[A]	GLU
1	1-J	455[A]	LEU
1	1-J	468[A]	PHE
1	1-J	470[A]	LYS
2	1-K	130[A]	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	1-K	137[A]	ASN
2	1-K	141[A]	LYS
2	1-K	150[A]	THR
2	1-K	162[A]	ASP
2	1-K	167[A]	VAL
2	1-L	131[A]	LEU
2	1-L	136[A]	ARG
2	1-L	141[A]	LYS
2	1-L	142[A]	HIS
2	1-L	144[A]	LEU
2	1-L	147[A]	SER
2	1-L	152[A]	THR
2	1-L	165[A]	LYS
2	1-L	169[A]	LEU
2	1-L	170[A]	LYS
2	1-L	171[A]	GLN
2	1-L	172[A]	THR
2	1-M	138[A]	ILE
2	1-M	142[A]	HIS
2	1-M	143[A]	SER
2	1-M	145[A]	ASP
2	1-M	150[A]	THR
2	1-M	157[A]	ILE
2	1-M	160[A]	LYS
2	1-M	170[A]	LYS
2	1-M	171[A]	GLN
2	1-N	145[A]	ASP
2	1-N	166[A]	LEU
2	1-N	168[A]	GLN
2	1-N	170[A]	LYS
2	1-N	171[A]	GLN
2	1-O	131[A]	LEU
2	1-O	132[A]	SER
2	1-O	138[A]	ILE
2	1-O	142[A]	HIS
2	1-O	144[A]	LEU
2	1-O	162[A]	ASP
2	1-O	165[A]	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (143) such sidechains are listed below:

Mol	Chain	Res	Type
1	1-A	38[A]	ASN
1	1-A	67[A]	HIS
1	1-A	84[A]	ASN
1	1-A	110[A]	ASN
1	1-A	137[A]	GLN
1	1-A	212[A]	HIS
1	1-A	225[A]	ASN
1	1-A	361[A]	HIS
1	1-A	397[A]	ASN
1	1-A	409[A]	GLN
1	1-A	430[A]	ASN
1	1-A	463[A]	ASN
1	1-B	38[A]	ASN
1	1-B	59[A]	ASN
1	1-B	91[A]	GLN
1	1-B	125[A]	ASN
1	1-B	126[A]	GLN
1	1-B	137[A]	GLN
1	1-B	286[A]	ASN
1	1-B	305[A]	ASN
1	1-B	329[A]	HIS
1	1-B	373[A]	GLN
1	1-B	397[A]	ASN
1	1-B	409[A]	GLN
1	1-B	450[A]	HIS
1	1-B	452[A]	HIS
1	1-C	3[A]	GLN
1	1-C	38[A]	ASN
1	1-C	59[A]	ASN
1	1-C	137[A]	GLN
1	1-C	233[A]	GLN
1	1-C	240[A]	ASN
1	1-C	309[A]	GLN
1	1-C	352[A]	ASN
1	1-C	361[A]	HIS
1	1-C	397[A]	ASN
1	1-C	409[A]	GLN
1	1-C	430[A]	ASN
1	1-C	463[A]	ASN
1	1-D	3[A]	GLN
1	1-D	27[A]	GLN
1	1-D	38[A]	ASN
1	1-D	110[A]	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	1-D	143[A]	ASN
1	1-D	225[A]	ASN
1	1-D	231[A]	GLN
1	1-D	233[A]	GLN
1	1-D	286[A]	ASN
1	1-D	305[A]	ASN
1	1-D	348[A]	HIS
1	1-D	409[A]	GLN
1	1-D	419[A]	HIS
1	1-D	430[A]	ASN
1	1-D	450[A]	HIS
1	1-E	84[A]	ASN
1	1-E	109[A]	GLN
1	1-E	110[A]	ASN
1	1-E	116[A]	ASN
1	1-E	137[A]	GLN
1	1-E	143[A]	ASN
1	1-E	231[A]	GLN
1	1-E	305[A]	ASN
1	1-E	309[A]	GLN
1	1-E	314[A]	ASN
1	1-E	361[A]	HIS
1	1-E	409[A]	GLN
1	1-E	419[A]	HIS
1	1-E	430[A]	ASN
1	1-E	463[A]	ASN
1	1-F	3[A]	GLN
1	1-F	27[A]	GLN
1	1-F	38[A]	ASN
1	1-F	84[A]	ASN
1	1-F	91[A]	GLN
1	1-F	116[A]	ASN
1	1-F	137[A]	GLN
1	1-F	143[A]	ASN
1	1-F	231[A]	GLN
1	1-F	233[A]	GLN
1	1-F	286[A]	ASN
1	1-F	314[A]	ASN
1	1-F	348[A]	HIS
1	1-F	373[A]	GLN
1	1-F	397[A]	ASN
1	1-F	430[A]	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	1-F	450[A]	HIS
1	1-G	84[A]	ASN
1	1-G	110[A]	ASN
1	1-G	125[A]	ASN
1	1-G	137[A]	GLN
1	1-G	233[A]	GLN
1	1-G	286[A]	ASN
1	1-G	309[A]	GLN
1	1-G	314[A]	ASN
1	1-G	352[A]	ASN
1	1-G	409[A]	GLN
1	1-G	430[A]	ASN
1	1-G	450[A]	HIS
1	1-G	463[A]	ASN
1	1-H	27[A]	GLN
1	1-H	59[A]	ASN
1	1-H	91[A]	GLN
1	1-H	137[A]	GLN
1	1-H	225[A]	ASN
1	1-H	305[A]	ASN
1	1-H	373[A]	GLN
1	1-H	397[A]	ASN
1	1-H	450[A]	HIS
1	1-H	473[A]	ASN
1	1-I	27[A]	GLN
1	1-I	110[A]	ASN
1	1-I	126[A]	GLN
1	1-I	225[A]	ASN
1	1-I	231[A]	GLN
1	1-I	233[A]	GLN
1	1-I	286[A]	ASN
1	1-I	309[A]	GLN
1	1-I	352[A]	ASN
1	1-I	409[A]	GLN
1	1-I	430[A]	ASN
1	1-I	463[A]	ASN
1	1-J	27[A]	GLN
1	1-J	38[A]	ASN
1	1-J	58[A]	ASN
1	1-J	59[A]	ASN
1	1-J	67[A]	HIS
1	1-J	91[A]	GLN

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Mol	Chain	Res	Type
1	1-J	109[A]	GLN
1	1-J	231[A]	GLN
1	1-J	305[A]	ASN
1	1-J	309[A]	GLN
1	1-J	352[A]	ASN
1	1-J	373[A]	GLN
1	1-J	397[A]	ASN
1	1-J	409[A]	GLN
2	1-K	137[A]	ASN
2	1-K	148[A]	GLN
2	1-L	168[A]	GLN
2	1-M	137[A]	ASN
2	1-M	142[A]	HIS
2	1-N	142[A]	HIS
2	1-N	168[A]	GLN
2	1-O	137[A]	ASN

#### 4.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

#### 4.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

#### 4.6 Ligand geometry [i](#)

20 ligands are modelled in this entry.

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	FAD	1-I	4758[A]	-	53,58,58	1.36	6 (11%)	68,89,89	1.83	16 (23%)
3	FAD	2-A	4751[C]	-	53,58,58	1.36	6 (11%)	68,89,89	1.83	16 (23%)
3	FAD	2-I	4759[C]	-	53,58,58	1.36	6 (11%)	68,89,89	1.83	16 (23%)
3	FAD	1-G	4756[A]	-	53,58,58	1.32	8 (15%)	68,89,89	1.45	12 (17%)
3	FAD	2-D	4754[C]	-	53,58,58	1.36	6 (11%)	68,89,89	1.83	16 (23%)
3	FAD	2-G	4757[C]	-	53,58,58	1.53	10 (18%)	68,89,89	1.61	11 (16%)
3	FAD	2-C	4753[C]	-	53,58,58	1.34	5 (9%)	68,89,89	1.43	6 (8%)
3	FAD	1-F	4755[A]	-	53,58,58	1.35	6 (11%)	68,89,89	1.83	16 (23%)
4	FAD	1-J	4759[A]	-	53,58,58	1.36	6 (11%)	68,89,89	1.83	16 (23%)
3	FAD	2-E	4755[C]	-	53,58,58	1.35	6 (11%)	68,89,89	1.83	16 (23%)
3	FAD	1-E	4754[A]	-	53,58,58	1.36	6 (11%)	68,89,89	1.83	16 (23%)
3	FAD	2-B	4752[C]	-	53,58,58	1.36	6 (11%)	68,89,89	1.83	16 (23%)
3	FAD	1-A	4750[A]	-	53,58,58	1.36	6 (11%)	68,89,89	1.83	16 (23%)
3	FAD	1-B	4751[A]	-	53,58,58	1.36	6 (11%)	68,89,89	1.83	16 (23%)
3	FAD	2-F	4756[C]	-	53,58,58	1.32	8 (15%)	68,89,89	1.45	12 (17%)
3	FAD	1-H	4757[A]	-	53,58,58	1.53	10 (18%)	68,89,89	1.61	11 (16%)
3	FAD	2-O	4750[C]	-	53,58,58	1.36	6 (11%)	68,89,89	1.83	16 (23%)
3	FAD	1-C	4752[A]	-	53,58,58	1.36	6 (11%)	68,89,89	1.83	16 (23%)
3	FAD	1-D	4753[A]	-	53,58,58	1.34	5 (9%)	68,89,89	1.43	6 (8%)
3	FAD	2-H	4758[C]	-	53,58,58	1.36	6 (11%)	68,89,89	1.83	16 (23%)

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	FAD	1-I	4758[A]	-	-	2/30/50/50	0/6/6/6
3	FAD	2-A	4751[C]	-	-	2/30/50/50	0/6/6/6
3	FAD	2-I	4759[C]	-	-	2/30/50/50	0/6/6/6
3	FAD	1-G	4756[A]	-	-	3/30/50/50	0/6/6/6
3	FAD	2-D	4754[C]	-	-	2/30/50/50	0/6/6/6
3	FAD	2-G	4757[C]	-	-	2/30/50/50	0/6/6/6
3	FAD	2-C	4753[C]	-	-	4/30/50/50	0/6/6/6
3	FAD	1-F	4755[A]	-	-	2/30/50/50	0/6/6/6
4	FAD	1-J	4759[A]	-	-	2/30/50/50	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FAD	2-E	4755[C]	-	-	2/30/50/50	0/6/6/6
3	FAD	1-E	4754[A]	-	-	2/30/50/50	0/6/6/6
3	FAD	2-B	4752[C]	-	-	2/30/50/50	0/6/6/6
3	FAD	1-A	4750[A]	-	-	2/30/50/50	0/6/6/6
3	FAD	1-B	4751[A]	-	-	2/30/50/50	0/6/6/6
3	FAD	2-F	4756[C]	-	-	3/30/50/50	0/6/6/6
3	FAD	1-H	4757[A]	-	-	2/30/50/50	0/6/6/6
3	FAD	2-O	4750[C]	-	-	2/30/50/50	0/6/6/6
3	FAD	1-C	4752[A]	-	-	2/30/50/50	0/6/6/6
3	FAD	1-D	4753[A]	-	-	4/30/50/50	0/6/6/6
3	FAD	2-H	4758[C]	-	-	2/30/50/50	0/6/6/6

All (130) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	2-G	4757[C]	FAD	C2A-N3A	4.35	1.39	1.32
3	1-H	4757[A]	FAD	C2A-N3A	4.35	1.39	1.32
3	2-G	4757[C]	FAD	C4X-N5	4.30	1.39	1.30
3	1-H	4757[A]	FAD	C4X-N5	4.30	1.39	1.30
3	2-H	4758[C]	FAD	C4X-N5	4.28	1.39	1.30
3	1-I	4758[A]	FAD	C4X-N5	4.28	1.39	1.30
3	2-I	4759[C]	FAD	C4X-N5	4.28	1.39	1.30
4	1-J	4759[A]	FAD	C4X-N5	4.28	1.39	1.30
3	1-A	4750[A]	FAD	C4X-N5	4.27	1.39	1.30
3	2-O	4750[C]	FAD	C4X-N5	4.27	1.39	1.30
3	2-A	4751[C]	FAD	C4X-N5	4.27	1.39	1.30
3	1-B	4751[A]	FAD	C4X-N5	4.27	1.39	1.30
3	2-B	4752[C]	FAD	C4X-N5	4.26	1.39	1.30
3	1-C	4752[A]	FAD	C4X-N5	4.26	1.39	1.30
3	2-D	4754[C]	FAD	C4X-N5	4.24	1.39	1.30
3	1-E	4754[A]	FAD	C4X-N5	4.24	1.39	1.30
3	2-E	4755[C]	FAD	C4X-N5	4.21	1.38	1.30
3	1-F	4755[A]	FAD	C4X-N5	4.21	1.38	1.30
3	2-F	4756[C]	FAD	C2A-N3A	3.85	1.38	1.32
3	1-G	4756[A]	FAD	C2A-N3A	3.85	1.38	1.32
3	2-C	4753[C]	FAD	C2A-N3A	3.51	1.37	1.32
3	1-D	4753[A]	FAD	C2A-N3A	3.51	1.37	1.32
3	2-G	4757[C]	FAD	C2B-C1B	-3.44	1.48	1.53
3	1-H	4757[A]	FAD	C2B-C1B	-3.44	1.48	1.53
3	2-H	4758[C]	FAD	C2B-C1B	-3.31	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	1-I	4758[A]	FAD	C2B-C1B	-3.31	1.48	1.53
3	2-A	4751[C]	FAD	C2B-C1B	-3.26	1.48	1.53
3	1-B	4751[A]	FAD	C2B-C1B	-3.26	1.48	1.53
3	2-B	4752[C]	FAD	C2B-C1B	-3.25	1.48	1.53
3	1-C	4752[A]	FAD	C2B-C1B	-3.25	1.48	1.53
3	1-A	4750[A]	FAD	C2B-C1B	-3.23	1.48	1.53
3	2-O	4750[C]	FAD	C2B-C1B	-3.23	1.48	1.53
3	2-D	4754[C]	FAD	C2B-C1B	-3.23	1.48	1.53
3	1-E	4754[A]	FAD	C2B-C1B	-3.23	1.48	1.53
3	2-E	4755[C]	FAD	C2B-C1B	-3.23	1.48	1.53
3	1-F	4755[A]	FAD	C2B-C1B	-3.23	1.48	1.53
3	2-I	4759[C]	FAD	C2B-C1B	-3.23	1.48	1.53
4	1-J	4759[A]	FAD	C2B-C1B	-3.23	1.48	1.53
3	2-F	4756[C]	FAD	O2'-C2'	-3.10	1.36	1.43
3	1-G	4756[A]	FAD	O2'-C2'	-3.10	1.36	1.43
3	2-E	4755[C]	FAD	C2A-N1A	2.90	1.39	1.33
3	1-F	4755[A]	FAD	C2A-N1A	2.90	1.39	1.33
3	2-A	4751[C]	FAD	C2A-N1A	2.89	1.39	1.33
3	1-B	4751[A]	FAD	C2A-N1A	2.89	1.39	1.33
3	1-A	4750[A]	FAD	C2A-N1A	2.88	1.39	1.33
3	2-O	4750[C]	FAD	C2A-N1A	2.88	1.39	1.33
3	2-I	4759[C]	FAD	C2A-N1A	2.88	1.39	1.33
4	1-J	4759[A]	FAD	C2A-N1A	2.88	1.39	1.33
3	2-B	4752[C]	FAD	C2A-N1A	2.87	1.39	1.33
3	1-C	4752[A]	FAD	C2A-N1A	2.87	1.39	1.33
3	2-D	4754[C]	FAD	C2A-N1A	2.86	1.39	1.33
3	1-E	4754[A]	FAD	C2A-N1A	2.86	1.39	1.33
3	2-C	4753[C]	FAD	C4X-N5	2.85	1.36	1.30
3	1-D	4753[A]	FAD	C4X-N5	2.85	1.36	1.30
3	2-H	4758[C]	FAD	C2A-N1A	2.85	1.39	1.33
3	1-I	4758[A]	FAD	C2A-N1A	2.85	1.39	1.33
3	2-G	4757[C]	FAD	O4'-C4'	-2.84	1.37	1.43
3	1-H	4757[A]	FAD	O4'-C4'	-2.84	1.37	1.43
3	2-C	4753[C]	FAD	C2B-C1B	-2.63	1.49	1.53
3	1-D	4753[A]	FAD	C2B-C1B	-2.63	1.49	1.53
3	2-G	4757[C]	FAD	O4B-C4B	-2.57	1.39	1.45
3	1-H	4757[A]	FAD	O4B-C4B	-2.57	1.39	1.45
3	2-F	4756[C]	FAD	C10-N1	2.52	1.38	1.33
3	1-G	4756[A]	FAD	C10-N1	2.52	1.38	1.33
3	2-F	4756[C]	FAD	C9A-N10	-2.40	1.36	1.41
3	1-G	4756[A]	FAD	C9A-N10	-2.40	1.36	1.41
3	2-G	4757[C]	FAD	C4'-C3'	-2.38	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	1-H	4757[A]	FAD	C4'-C3'	-2.38	1.49	1.53
3	2-F	4756[C]	FAD	C4X-N5	2.37	1.35	1.30
3	1-G	4756[A]	FAD	C4X-N5	2.37	1.35	1.30
3	2-D	4754[C]	FAD	C10-N1	2.31	1.37	1.33
3	1-E	4754[A]	FAD	C10-N1	2.31	1.37	1.33
3	2-I	4759[C]	FAD	C10-N1	2.31	1.37	1.33
4	1-J	4759[A]	FAD	C10-N1	2.31	1.37	1.33
3	2-C	4753[C]	FAD	C5'-C4'	2.31	1.55	1.51
3	1-D	4753[A]	FAD	C5'-C4'	2.31	1.55	1.51
3	2-I	4759[C]	FAD	C6A-C5A	-2.30	1.34	1.43
4	1-J	4759[A]	FAD	C6A-C5A	-2.30	1.34	1.43
3	2-F	4756[C]	FAD	C2A-N1A	2.29	1.38	1.33
3	1-G	4756[A]	FAD	C2A-N1A	2.29	1.38	1.33
3	2-D	4754[C]	FAD	C6A-C5A	-2.29	1.34	1.43
3	1-E	4754[A]	FAD	C6A-C5A	-2.29	1.34	1.43
3	2-A	4751[C]	FAD	C10-N1	2.28	1.37	1.33
3	1-B	4751[A]	FAD	C10-N1	2.28	1.37	1.33
3	2-G	4757[C]	FAD	P-O1P	-2.28	1.42	1.50
3	1-H	4757[A]	FAD	P-O1P	-2.28	1.42	1.50
3	2-B	4752[C]	FAD	C6A-C5A	-2.28	1.34	1.43
3	1-C	4752[A]	FAD	C6A-C5A	-2.28	1.34	1.43
3	2-B	4752[C]	FAD	C10-N1	2.28	1.37	1.33
3	1-C	4752[A]	FAD	C10-N1	2.28	1.37	1.33
3	1-A	4750[A]	FAD	C10-N1	2.28	1.37	1.33
3	2-O	4750[C]	FAD	C10-N1	2.28	1.37	1.33
3	1-A	4750[A]	FAD	C6A-C5A	-2.28	1.34	1.43
3	2-O	4750[C]	FAD	C6A-C5A	-2.28	1.34	1.43
3	2-I	4759[C]	FAD	C4X-C10	-2.27	1.37	1.44
4	1-J	4759[A]	FAD	C4X-C10	-2.27	1.37	1.44
3	2-H	4758[C]	FAD	C6A-C5A	-2.27	1.34	1.43
3	1-I	4758[A]	FAD	C6A-C5A	-2.27	1.34	1.43
3	2-E	4755[C]	FAD	C10-N1	2.27	1.37	1.33
3	1-F	4755[A]	FAD	C10-N1	2.27	1.37	1.33
3	2-E	4755[C]	FAD	C6A-C5A	-2.26	1.34	1.43
3	1-F	4755[A]	FAD	C6A-C5A	-2.26	1.34	1.43
3	2-A	4751[C]	FAD	C4X-C10	-2.26	1.37	1.44
3	1-B	4751[A]	FAD	C4X-C10	-2.26	1.37	1.44
3	2-A	4751[C]	FAD	C6A-C5A	-2.26	1.34	1.43
3	1-B	4751[A]	FAD	C6A-C5A	-2.26	1.34	1.43
3	2-H	4758[C]	FAD	C10-N1	2.26	1.37	1.33
3	1-I	4758[A]	FAD	C10-N1	2.26	1.37	1.33
3	1-A	4750[A]	FAD	C4X-C10	-2.25	1.37	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	2-O	4750[C]	FAD	C4X-C10	-2.25	1.37	1.44
3	2-G	4757[C]	FAD	C9A-N10	-2.25	1.37	1.41
3	1-H	4757[A]	FAD	C9A-N10	-2.25	1.37	1.41
3	2-D	4754[C]	FAD	C4X-C10	-2.24	1.37	1.44
3	1-E	4754[A]	FAD	C4X-C10	-2.24	1.37	1.44
3	2-H	4758[C]	FAD	C4X-C10	-2.24	1.37	1.44
3	1-I	4758[A]	FAD	C4X-C10	-2.24	1.37	1.44
3	2-B	4752[C]	FAD	C4X-C10	-2.24	1.37	1.44
3	1-C	4752[A]	FAD	C4X-C10	-2.24	1.37	1.44
3	2-E	4755[C]	FAD	C4X-C10	-2.22	1.37	1.44
3	1-F	4755[A]	FAD	C4X-C10	-2.22	1.37	1.44
3	2-G	4757[C]	FAD	C10-N1	2.15	1.37	1.33
3	1-H	4757[A]	FAD	C10-N1	2.15	1.37	1.33
3	2-G	4757[C]	FAD	C5A-C4A	-2.14	1.35	1.40
3	1-H	4757[A]	FAD	C5A-C4A	-2.14	1.35	1.40
3	2-F	4756[C]	FAD	O2-C2	-2.06	1.20	1.24
3	1-G	4756[A]	FAD	O2-C2	-2.06	1.20	1.24
3	2-C	4753[C]	FAD	C9A-C5X	-2.06	1.37	1.41
3	1-D	4753[A]	FAD	C9A-C5X	-2.06	1.37	1.41
3	2-F	4756[C]	FAD	C2B-C1B	-2.01	1.50	1.53
3	1-G	4756[A]	FAD	C2B-C1B	-2.01	1.50	1.53

All (282) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	1-A	4750[A]	FAD	N3A-C2A-N1A	-7.14	117.53	128.68
3	2-O	4750[C]	FAD	N3A-C2A-N1A	-7.14	117.53	128.68
3	2-E	4755[C]	FAD	N3A-C2A-N1A	-7.13	117.54	128.68
3	1-F	4755[A]	FAD	N3A-C2A-N1A	-7.13	117.54	128.68
3	2-A	4751[C]	FAD	N3A-C2A-N1A	-7.12	117.55	128.68
3	1-B	4751[A]	FAD	N3A-C2A-N1A	-7.12	117.55	128.68
3	2-I	4759[C]	FAD	N3A-C2A-N1A	-7.12	117.55	128.68
4	1-J	4759[A]	FAD	N3A-C2A-N1A	-7.12	117.55	128.68
3	2-B	4752[C]	FAD	N3A-C2A-N1A	-7.12	117.56	128.68
3	1-C	4752[A]	FAD	N3A-C2A-N1A	-7.12	117.56	128.68
3	2-D	4754[C]	FAD	N3A-C2A-N1A	-7.10	117.58	128.68
3	1-E	4754[A]	FAD	N3A-C2A-N1A	-7.10	117.58	128.68
3	2-H	4758[C]	FAD	N3A-C2A-N1A	-7.08	117.62	128.68
3	1-I	4758[A]	FAD	N3A-C2A-N1A	-7.08	117.62	128.68
3	2-G	4757[C]	FAD	N3A-C2A-N1A	-5.99	119.31	128.68
3	1-H	4757[A]	FAD	N3A-C2A-N1A	-5.99	119.31	128.68
3	2-C	4753[C]	FAD	N3A-C2A-N1A	-5.90	119.46	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	1-D	4753[A]	FAD	N3A-C2A-N1A	-5.90	119.46	128.68
3	2-F	4756[C]	FAD	N3A-C2A-N1A	-5.74	119.71	128.68
3	1-G	4756[A]	FAD	N3A-C2A-N1A	-5.74	119.71	128.68
3	2-C	4753[C]	FAD	C4X-C10-N10	4.01	122.35	116.48
3	1-D	4753[A]	FAD	C4X-C10-N10	4.01	122.35	116.48
3	2-I	4759[C]	FAD	O3B-C3B-C4B	-3.96	99.60	111.05
4	1-J	4759[A]	FAD	O3B-C3B-C4B	-3.96	99.60	111.05
3	2-D	4754[C]	FAD	O3B-C3B-C4B	-3.96	99.60	111.05
3	1-E	4754[A]	FAD	O3B-C3B-C4B	-3.96	99.60	111.05
3	2-B	4752[C]	FAD	O3B-C3B-C4B	-3.96	99.61	111.05
3	1-C	4752[A]	FAD	O3B-C3B-C4B	-3.96	99.61	111.05
3	1-A	4750[A]	FAD	O3B-C3B-C4B	-3.95	99.62	111.05
3	2-O	4750[C]	FAD	O3B-C3B-C4B	-3.95	99.62	111.05
3	2-A	4751[C]	FAD	O3B-C3B-C4B	-3.95	99.63	111.05
3	1-B	4751[A]	FAD	O3B-C3B-C4B	-3.95	99.63	111.05
3	2-H	4758[C]	FAD	O3B-C3B-C4B	-3.95	99.64	111.05
3	1-I	4758[A]	FAD	O3B-C3B-C4B	-3.95	99.64	111.05
3	2-E	4755[C]	FAD	O3B-C3B-C4B	-3.95	99.64	111.05
3	1-F	4755[A]	FAD	O3B-C3B-C4B	-3.95	99.64	111.05
3	2-G	4757[C]	FAD	O4B-C1B-C2B	-3.67	101.57	106.93
3	1-H	4757[A]	FAD	O4B-C1B-C2B	-3.67	101.57	106.93
3	2-G	4757[C]	FAD	C4X-C10-N10	3.65	121.82	116.48
3	1-H	4757[A]	FAD	C4X-C10-N10	3.65	121.82	116.48
3	2-H	4758[C]	FAD	C9A-C5X-N5	-3.41	118.72	122.43
3	1-I	4758[A]	FAD	C9A-C5X-N5	-3.41	118.72	122.43
3	2-D	4754[C]	FAD	C9A-C5X-N5	-3.41	118.73	122.43
3	1-E	4754[A]	FAD	C9A-C5X-N5	-3.41	118.73	122.43
3	1-A	4750[A]	FAD	C9A-C5X-N5	-3.40	118.74	122.43
3	2-O	4750[C]	FAD	C9A-C5X-N5	-3.40	118.74	122.43
3	2-B	4752[C]	FAD	C9A-C5X-N5	-3.40	118.74	122.43
3	1-C	4752[A]	FAD	C9A-C5X-N5	-3.40	118.74	122.43
3	2-E	4755[C]	FAD	C9A-C5X-N5	-3.39	118.75	122.43
3	1-F	4755[A]	FAD	C9A-C5X-N5	-3.39	118.75	122.43
3	2-I	4759[C]	FAD	C9A-C5X-N5	-3.39	118.75	122.43
4	1-J	4759[A]	FAD	C9A-C5X-N5	-3.39	118.75	122.43
3	2-A	4751[C]	FAD	C9A-C5X-N5	-3.37	118.77	122.43
3	1-B	4751[A]	FAD	C9A-C5X-N5	-3.37	118.77	122.43
3	1-A	4750[A]	FAD	C2A-N1A-C6A	3.27	124.35	118.75
3	2-O	4750[C]	FAD	C2A-N1A-C6A	3.27	124.35	118.75
3	2-A	4751[C]	FAD	C2A-N1A-C6A	3.26	124.33	118.75
3	1-B	4751[A]	FAD	C2A-N1A-C6A	3.26	124.33	118.75
3	2-E	4755[C]	FAD	C4X-C4-N3	3.26	121.47	113.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	1-F	4755[A]	FAD	C4X-C4-N3	3.26	121.47	113.19
3	2-I	4759[C]	FAD	C2A-N1A-C6A	3.25	124.32	118.75
4	1-J	4759[A]	FAD	C2A-N1A-C6A	3.25	124.32	118.75
3	2-B	4752[C]	FAD	C2A-N1A-C6A	3.25	124.31	118.75
3	1-C	4752[A]	FAD	C2A-N1A-C6A	3.25	124.31	118.75
3	2-I	4759[C]	FAD	C4X-C4-N3	3.25	121.44	113.19
4	1-J	4759[A]	FAD	C4X-C4-N3	3.25	121.44	113.19
3	2-H	4758[C]	FAD	C2A-N1A-C6A	3.25	124.31	118.75
3	1-I	4758[A]	FAD	C2A-N1A-C6A	3.25	124.31	118.75
3	2-A	4751[C]	FAD	C4X-C4-N3	3.25	121.43	113.19
3	1-B	4751[A]	FAD	C4X-C4-N3	3.25	121.43	113.19
3	2-H	4758[C]	FAD	C4X-C4-N3	3.24	121.43	113.19
3	1-I	4758[A]	FAD	C4X-C4-N3	3.24	121.43	113.19
3	2-B	4752[C]	FAD	C4X-C4-N3	3.24	121.43	113.19
3	1-C	4752[A]	FAD	C4X-C4-N3	3.24	121.43	113.19
3	1-A	4750[A]	FAD	C4X-C4-N3	3.24	121.42	113.19
3	2-O	4750[C]	FAD	C4X-C4-N3	3.24	121.42	113.19
3	2-E	4755[C]	FAD	C2A-N1A-C6A	3.24	124.30	118.75
3	1-F	4755[A]	FAD	C2A-N1A-C6A	3.24	124.30	118.75
3	2-D	4754[C]	FAD	C2A-N1A-C6A	3.23	124.28	118.75
3	1-E	4754[A]	FAD	C2A-N1A-C6A	3.23	124.28	118.75
3	2-D	4754[C]	FAD	C4X-C4-N3	3.22	121.37	113.19
3	1-E	4754[A]	FAD	C4X-C4-N3	3.22	121.37	113.19
3	2-I	4759[C]	FAD	C4-N3-C2	-3.13	119.86	125.64
4	1-J	4759[A]	FAD	C4-N3-C2	-3.13	119.86	125.64
3	2-E	4755[C]	FAD	C4-N3-C2	-3.13	119.86	125.64
3	1-F	4755[A]	FAD	C4-N3-C2	-3.13	119.86	125.64
3	2-A	4751[C]	FAD	C4-N3-C2	-3.12	119.87	125.64
3	1-B	4751[A]	FAD	C4-N3-C2	-3.12	119.87	125.64
3	1-A	4750[A]	FAD	C4-N3-C2	-3.12	119.87	125.64
3	2-O	4750[C]	FAD	C4-N3-C2	-3.12	119.87	125.64
3	2-B	4752[C]	FAD	C4-N3-C2	-3.12	119.88	125.64
3	1-C	4752[A]	FAD	C4-N3-C2	-3.12	119.88	125.64
3	2-H	4758[C]	FAD	C4-N3-C2	-3.12	119.88	125.64
3	1-I	4758[A]	FAD	C4-N3-C2	-3.12	119.88	125.64
3	2-G	4757[C]	FAD	C4-N3-C2	-3.11	119.90	125.64
3	1-H	4757[A]	FAD	C4-N3-C2	-3.11	119.90	125.64
3	2-D	4754[C]	FAD	C4-N3-C2	-3.10	119.91	125.64
3	1-E	4754[A]	FAD	C4-N3-C2	-3.10	119.91	125.64
3	2-D	4754[C]	FAD	C1B-N9A-C4A	-3.10	121.19	126.64
3	1-E	4754[A]	FAD	C1B-N9A-C4A	-3.10	121.19	126.64
3	2-I	4759[C]	FAD	C1B-N9A-C4A	-3.10	121.19	126.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	1-J	4759[A]	FAD	C1B-N9A-C4A	-3.10	121.19	126.64
3	2-E	4755[C]	FAD	C1B-N9A-C4A	-3.09	121.21	126.64
3	1-F	4755[A]	FAD	C1B-N9A-C4A	-3.09	121.21	126.64
3	2-B	4752[C]	FAD	C1B-N9A-C4A	-3.08	121.22	126.64
3	1-C	4752[A]	FAD	C1B-N9A-C4A	-3.08	121.22	126.64
3	2-H	4758[C]	FAD	C1B-N9A-C4A	-3.07	121.25	126.64
3	1-I	4758[A]	FAD	C1B-N9A-C4A	-3.07	121.25	126.64
3	2-A	4751[C]	FAD	C1B-N9A-C4A	-3.07	121.25	126.64
3	1-B	4751[A]	FAD	C1B-N9A-C4A	-3.07	121.25	126.64
3	1-A	4750[A]	FAD	C1B-N9A-C4A	-3.06	121.27	126.64
3	2-O	4750[C]	FAD	C1B-N9A-C4A	-3.06	121.27	126.64
3	2-F	4756[C]	FAD	C4-N3-C2	-3.06	119.99	125.64
3	1-G	4756[A]	FAD	C4-N3-C2	-3.06	119.99	125.64
3	2-G	4757[C]	FAD	C4X-C4-N3	3.00	120.80	113.19
3	1-H	4757[A]	FAD	C4X-C4-N3	3.00	120.80	113.19
3	2-D	4754[C]	FAD	C5X-C9A-N10	2.94	120.99	117.95
3	1-E	4754[A]	FAD	C5X-C9A-N10	2.94	120.99	117.95
3	2-H	4758[C]	FAD	C5X-C9A-N10	2.93	120.98	117.95
3	1-I	4758[A]	FAD	C5X-C9A-N10	2.93	120.98	117.95
3	2-A	4751[C]	FAD	C5X-C9A-N10	2.93	120.98	117.95
3	1-B	4751[A]	FAD	C5X-C9A-N10	2.93	120.98	117.95
3	2-B	4752[C]	FAD	C5X-C9A-N10	2.92	120.97	117.95
3	1-C	4752[A]	FAD	C5X-C9A-N10	2.92	120.97	117.95
3	2-F	4756[C]	FAD	C4'-C3'-C2'	-2.92	107.28	113.36
3	1-G	4756[A]	FAD	C4'-C3'-C2'	-2.92	107.28	113.36
3	1-A	4750[A]	FAD	C5X-C9A-N10	2.91	120.96	117.95
3	2-O	4750[C]	FAD	C5X-C9A-N10	2.91	120.96	117.95
3	2-I	4759[C]	FAD	C5X-C9A-N10	2.90	120.95	117.95
4	1-J	4759[A]	FAD	C5X-C9A-N10	2.90	120.95	117.95
3	2-E	4755[C]	FAD	C5X-C9A-N10	2.88	120.93	117.95
3	1-F	4755[A]	FAD	C5X-C9A-N10	2.88	120.93	117.95
3	2-F	4756[C]	FAD	C4X-C10-N10	2.84	120.63	116.48
3	1-G	4756[A]	FAD	C4X-C10-N10	2.84	120.63	116.48
3	2-C	4753[C]	FAD	C10-C4X-N5	-2.80	118.92	124.86
3	1-D	4753[A]	FAD	C10-C4X-N5	-2.80	118.92	124.86
3	2-H	4758[C]	FAD	N6A-C6A-N1A	2.69	124.16	118.57
3	1-I	4758[A]	FAD	N6A-C6A-N1A	2.69	124.16	118.57
3	1-A	4750[A]	FAD	N6A-C6A-N1A	2.68	124.14	118.57
3	2-O	4750[C]	FAD	N6A-C6A-N1A	2.68	124.14	118.57
3	2-E	4755[C]	FAD	N6A-C6A-N1A	2.67	124.12	118.57
3	1-F	4755[A]	FAD	N6A-C6A-N1A	2.67	124.12	118.57
3	2-A	4751[C]	FAD	N6A-C6A-N1A	2.67	124.12	118.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	1-B	4751[A]	FAD	N6A-C6A-N1A	2.67	124.12	118.57
3	2-D	4754[C]	FAD	N6A-C6A-N1A	2.67	124.12	118.57
3	1-E	4754[A]	FAD	N6A-C6A-N1A	2.67	124.12	118.57
3	2-B	4752[C]	FAD	N6A-C6A-N1A	2.67	124.11	118.57
3	1-C	4752[A]	FAD	N6A-C6A-N1A	2.67	124.11	118.57
3	2-I	4759[C]	FAD	N6A-C6A-N1A	2.67	124.11	118.57
4	1-J	4759[A]	FAD	N6A-C6A-N1A	2.67	124.11	118.57
3	2-G	4757[C]	FAD	O4'-C4'-C3'	-2.65	102.65	109.10
3	1-H	4757[A]	FAD	O4'-C4'-C3'	-2.65	102.65	109.10
3	2-A	4751[C]	FAD	C4A-C5A-N7A	2.63	112.14	109.40
3	1-B	4751[A]	FAD	C4A-C5A-N7A	2.63	112.14	109.40
3	2-B	4752[C]	FAD	C4A-C5A-N7A	2.63	112.14	109.40
3	1-C	4752[A]	FAD	C4A-C5A-N7A	2.63	112.14	109.40
3	2-E	4755[C]	FAD	C4A-C5A-N7A	2.63	112.14	109.40
3	1-F	4755[A]	FAD	C4A-C5A-N7A	2.63	112.14	109.40
3	2-I	4759[C]	FAD	C4A-C5A-N7A	2.62	112.13	109.40
4	1-J	4759[A]	FAD	C4A-C5A-N7A	2.62	112.13	109.40
3	2-D	4754[C]	FAD	C4A-C5A-N7A	2.62	112.13	109.40
3	1-E	4754[A]	FAD	C4A-C5A-N7A	2.62	112.13	109.40
3	2-H	4758[C]	FAD	C4A-C5A-N7A	2.62	112.12	109.40
3	1-I	4758[A]	FAD	C4A-C5A-N7A	2.62	112.12	109.40
3	2-G	4757[C]	FAD	C10-C4X-N5	-2.61	119.31	124.86
3	1-H	4757[A]	FAD	C10-C4X-N5	-2.61	119.31	124.86
3	1-A	4750[A]	FAD	C4A-C5A-N7A	2.59	112.10	109.40
3	2-O	4750[C]	FAD	C4A-C5A-N7A	2.59	112.10	109.40
3	2-H	4758[C]	FAD	C10-N1-C2	2.51	121.91	116.90
3	1-I	4758[A]	FAD	C10-N1-C2	2.51	121.91	116.90
3	2-B	4752[C]	FAD	C10-N1-C2	2.50	121.90	116.90
3	1-C	4752[A]	FAD	C10-N1-C2	2.50	121.90	116.90
3	2-E	4755[C]	FAD	C10-N1-C2	2.50	121.89	116.90
3	1-F	4755[A]	FAD	C10-N1-C2	2.50	121.89	116.90
3	2-C	4753[C]	FAD	C4-C4X-C10	2.49	120.98	116.79
3	1-D	4753[A]	FAD	C4-C4X-C10	2.49	120.98	116.79
3	2-G	4757[C]	FAD	C4-C4X-N5	2.49	121.77	118.23
3	1-H	4757[A]	FAD	C4-C4X-N5	2.49	121.77	118.23
3	2-I	4759[C]	FAD	C10-N1-C2	2.49	121.87	116.90
4	1-J	4759[A]	FAD	C10-N1-C2	2.49	121.87	116.90
3	2-D	4754[C]	FAD	C10-N1-C2	2.48	121.86	116.90
3	1-E	4754[A]	FAD	C10-N1-C2	2.48	121.86	116.90
3	1-A	4750[A]	FAD	C10-N1-C2	2.48	121.86	116.90
3	2-O	4750[C]	FAD	C10-N1-C2	2.48	121.86	116.90
3	2-A	4751[C]	FAD	C10-N1-C2	2.48	121.85	116.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	1-B	4751[A]	FAD	C10-N1-C2	2.48	121.85	116.90
3	2-F	4756[C]	FAD	O4-C4-C4X	-2.46	120.07	126.60
3	1-G	4756[A]	FAD	O4-C4-C4X	-2.46	120.07	126.60
3	2-F	4756[C]	FAD	C4X-C4-N3	2.41	119.30	113.19
3	1-G	4756[A]	FAD	C4X-C4-N3	2.41	119.30	113.19
3	2-F	4756[C]	FAD	C4X-C10-N1	-2.40	119.16	124.73
3	1-G	4756[A]	FAD	C4X-C10-N1	-2.40	119.16	124.73
3	2-F	4756[C]	FAD	O2'-C2'-C3'	-2.39	103.29	109.10
3	1-G	4756[A]	FAD	O2'-C2'-C3'	-2.39	103.29	109.10
3	2-D	4754[C]	FAD	C4X-C10-N10	2.36	119.92	116.48
3	1-E	4754[A]	FAD	C4X-C10-N10	2.36	119.92	116.48
3	2-A	4751[C]	FAD	C4X-C10-N10	2.35	119.92	116.48
3	1-B	4751[A]	FAD	C4X-C10-N10	2.35	119.92	116.48
3	2-I	4759[C]	FAD	C4X-C10-N10	2.35	119.92	116.48
4	1-J	4759[A]	FAD	C4X-C10-N10	2.35	119.92	116.48
3	2-B	4752[C]	FAD	C4X-C10-N10	2.35	119.91	116.48
3	1-C	4752[A]	FAD	C4X-C10-N10	2.35	119.91	116.48
3	1-A	4750[A]	FAD	C4X-C10-N10	2.35	119.91	116.48
3	2-O	4750[C]	FAD	C4X-C10-N10	2.35	119.91	116.48
3	2-H	4758[C]	FAD	C4X-C10-N10	2.34	119.91	116.48
3	1-I	4758[A]	FAD	C4X-C10-N10	2.34	119.91	116.48
3	2-E	4755[C]	FAD	C4X-C10-N10	2.32	119.88	116.48
3	1-F	4755[A]	FAD	C4X-C10-N10	2.32	119.88	116.48
3	2-F	4756[C]	FAD	C10-C4X-N5	-2.31	119.96	124.86
3	1-G	4756[A]	FAD	C10-C4X-N5	-2.31	119.96	124.86
3	2-G	4757[C]	FAD	C5X-C9A-N10	2.26	120.29	117.95
3	1-H	4757[A]	FAD	C5X-C9A-N10	2.26	120.29	117.95
3	2-E	4755[C]	FAD	O2B-C2B-C1B	-2.25	102.53	110.85
3	1-F	4755[A]	FAD	O2B-C2B-C1B	-2.25	102.53	110.85
3	2-I	4759[C]	FAD	O2B-C2B-C1B	-2.25	102.53	110.85
4	1-J	4759[A]	FAD	O2B-C2B-C1B	-2.25	102.53	110.85
3	2-A	4751[C]	FAD	O2B-C2B-C1B	-2.25	102.56	110.85
3	1-B	4751[A]	FAD	O2B-C2B-C1B	-2.25	102.56	110.85
3	2-D	4754[C]	FAD	O2B-C2B-C1B	-2.25	102.56	110.85
3	1-E	4754[A]	FAD	O2B-C2B-C1B	-2.25	102.56	110.85
3	1-A	4750[A]	FAD	O2B-C2B-C1B	-2.24	102.57	110.85
3	2-O	4750[C]	FAD	O2B-C2B-C1B	-2.24	102.57	110.85
3	2-B	4752[C]	FAD	O2B-C2B-C1B	-2.24	102.58	110.85
3	1-C	4752[A]	FAD	O2B-C2B-C1B	-2.24	102.58	110.85
3	2-F	4756[C]	FAD	C8M-C8-C7	-2.24	116.15	120.74
3	1-G	4756[A]	FAD	C8M-C8-C7	-2.24	116.15	120.74
3	2-H	4758[C]	FAD	O2B-C2B-C1B	-2.24	102.59	110.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	1-I	4758[A]	FAD	O2B-C2B-C1B	-2.24	102.59	110.85
3	2-E	4755[C]	FAD	O4B-C1B-C2B	-2.22	103.68	106.93
3	1-F	4755[A]	FAD	O4B-C1B-C2B	-2.22	103.68	106.93
3	2-D	4754[C]	FAD	O4B-C1B-C2B	-2.20	103.71	106.93
3	1-E	4754[A]	FAD	O4B-C1B-C2B	-2.20	103.71	106.93
3	1-A	4750[A]	FAD	O4B-C1B-C2B	-2.20	103.71	106.93
3	2-O	4750[C]	FAD	O4B-C1B-C2B	-2.20	103.71	106.93
3	2-B	4752[C]	FAD	O4B-C1B-C2B	-2.20	103.71	106.93
3	1-C	4752[A]	FAD	O4B-C1B-C2B	-2.20	103.71	106.93
3	2-B	4752[C]	FAD	C4X-C10-N1	-2.19	119.64	124.73
3	1-C	4752[A]	FAD	C4X-C10-N1	-2.19	119.64	124.73
3	2-E	4755[C]	FAD	O4-C4-C4X	-2.19	120.79	126.60
3	1-F	4755[A]	FAD	O4-C4-C4X	-2.19	120.79	126.60
3	2-H	4758[C]	FAD	C4X-C10-N1	-2.19	119.65	124.73
3	1-I	4758[A]	FAD	C4X-C10-N1	-2.19	119.65	124.73
3	2-I	4759[C]	FAD	O4-C4-C4X	-2.19	120.79	126.60
4	1-J	4759[A]	FAD	O4-C4-C4X	-2.19	120.79	126.60
3	2-E	4755[C]	FAD	C4X-C10-N1	-2.19	119.66	124.73
3	1-F	4755[A]	FAD	C4X-C10-N1	-2.19	119.66	124.73
3	2-H	4758[C]	FAD	O4B-C1B-C2B	-2.19	103.73	106.93
3	1-I	4758[A]	FAD	O4B-C1B-C2B	-2.19	103.73	106.93
3	2-D	4754[C]	FAD	C4X-C10-N1	-2.19	119.66	124.73
3	1-E	4754[A]	FAD	C4X-C10-N1	-2.19	119.66	124.73
3	2-I	4759[C]	FAD	O4B-C1B-C2B	-2.18	103.73	106.93
4	1-J	4759[A]	FAD	O4B-C1B-C2B	-2.18	103.73	106.93
3	1-A	4750[A]	FAD	C4X-C10-N1	-2.18	119.66	124.73
3	2-O	4750[C]	FAD	C4X-C10-N1	-2.18	119.66	124.73
3	2-B	4752[C]	FAD	O4-C4-C4X	-2.18	120.81	126.60
3	1-C	4752[A]	FAD	O4-C4-C4X	-2.18	120.81	126.60
3	2-A	4751[C]	FAD	O4-C4-C4X	-2.18	120.81	126.60
3	1-B	4751[A]	FAD	O4-C4-C4X	-2.18	120.81	126.60
3	2-I	4759[C]	FAD	C4X-C10-N1	-2.18	119.67	124.73
4	1-J	4759[A]	FAD	C4X-C10-N1	-2.18	119.67	124.73
3	2-A	4751[C]	FAD	O4B-C1B-C2B	-2.18	103.74	106.93
3	1-B	4751[A]	FAD	O4B-C1B-C2B	-2.18	103.74	106.93
3	2-F	4756[C]	FAD	C4A-C5A-N7A	-2.18	107.13	109.40
3	1-G	4756[A]	FAD	C4A-C5A-N7A	-2.18	107.13	109.40
3	2-A	4751[C]	FAD	C4X-C10-N1	-2.18	119.68	124.73
3	1-B	4751[A]	FAD	C4X-C10-N1	-2.18	119.68	124.73
3	2-D	4754[C]	FAD	O4-C4-C4X	-2.17	120.84	126.60
3	1-E	4754[A]	FAD	O4-C4-C4X	-2.17	120.84	126.60
3	2-H	4758[C]	FAD	O4-C4-C4X	-2.17	120.84	126.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	1-I	4758[A]	FAD	O4-C4-C4X	-2.17	120.84	126.60
3	1-A	4750[A]	FAD	O4-C4-C4X	-2.17	120.84	126.60
3	2-O	4750[C]	FAD	O4-C4-C4X	-2.17	120.84	126.60
3	2-G	4757[C]	FAD	C4X-C10-N1	-2.16	119.71	124.73
3	1-H	4757[A]	FAD	C4X-C10-N1	-2.16	119.71	124.73
3	2-C	4753[C]	FAD	O4'-C4'-C5'	2.16	114.77	109.92
3	1-D	4753[A]	FAD	O4'-C4'-C5'	2.16	114.77	109.92
3	2-C	4753[C]	FAD	C4-N3-C2	-2.11	121.75	125.64
3	1-D	4753[A]	FAD	C4-N3-C2	-2.11	121.75	125.64
3	2-F	4756[C]	FAD	C4-C4X-C10	2.08	120.28	116.79
3	1-G	4756[A]	FAD	C4-C4X-C10	2.08	120.28	116.79
3	2-G	4757[C]	FAD	O4-C4-N3	-2.03	116.22	120.12
3	1-H	4757[A]	FAD	O4-C4-N3	-2.03	116.22	120.12

There are no chirality outliers.

All (46) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	1-A	4750[A]	FAD	PA-O3P-P-O5'
3	2-A	4751[C]	FAD	PA-O3P-P-O5'
3	1-B	4751[A]	FAD	PA-O3P-P-O5'
3	2-B	4752[C]	FAD	PA-O3P-P-O5'
3	1-C	4752[A]	FAD	PA-O3P-P-O5'
3	2-D	4754[C]	FAD	PA-O3P-P-O5'
3	1-E	4754[A]	FAD	PA-O3P-P-O5'
3	2-E	4755[C]	FAD	PA-O3P-P-O5'
3	1-F	4755[A]	FAD	PA-O3P-P-O5'
3	2-H	4758[C]	FAD	PA-O3P-P-O5'
3	1-I	4758[A]	FAD	PA-O3P-P-O5'
3	2-I	4759[C]	FAD	PA-O3P-P-O5'
4	1-J	4759[A]	FAD	PA-O3P-P-O5'
3	2-O	4750[C]	FAD	PA-O3P-P-O5'
3	2-C	4753[C]	FAD	O4B-C4B-C5B-O5B
3	1-D	4753[A]	FAD	O4B-C4B-C5B-O5B
3	2-C	4753[C]	FAD	C3B-C4B-C5B-O5B
3	1-D	4753[A]	FAD	C3B-C4B-C5B-O5B
3	2-F	4756[C]	FAD	O4B-C4B-C5B-O5B
3	1-G	4756[A]	FAD	O4B-C4B-C5B-O5B
3	2-C	4753[C]	FAD	PA-O3P-P-O5'
3	1-D	4753[A]	FAD	PA-O3P-P-O5'
3	2-F	4756[C]	FAD	PA-O3P-P-O5'
3	1-G	4756[A]	FAD	PA-O3P-P-O5'

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Mol	Chain	Res	Type	Atoms
3	2-G	4757[C]	FAD	PA-O3P-P-O5'
3	1-H	4757[A]	FAD	PA-O3P-P-O5'
3	2-G	4757[C]	FAD	O4B-C4B-C5B-O5B
3	1-H	4757[A]	FAD	O4B-C4B-C5B-O5B
3	2-F	4756[C]	FAD	C3B-C4B-C5B-O5B
3	1-G	4756[A]	FAD	C3B-C4B-C5B-O5B
3	1-A	4750[A]	FAD	O4B-C4B-C5B-O5B
3	2-A	4751[C]	FAD	O4B-C4B-C5B-O5B
3	1-B	4751[A]	FAD	O4B-C4B-C5B-O5B
3	2-B	4752[C]	FAD	O4B-C4B-C5B-O5B
3	1-C	4752[A]	FAD	O4B-C4B-C5B-O5B
3	2-D	4754[C]	FAD	O4B-C4B-C5B-O5B
3	1-E	4754[A]	FAD	O4B-C4B-C5B-O5B
3	2-E	4755[C]	FAD	O4B-C4B-C5B-O5B
3	1-F	4755[A]	FAD	O4B-C4B-C5B-O5B
3	2-H	4758[C]	FAD	O4B-C4B-C5B-O5B
3	1-I	4758[A]	FAD	O4B-C4B-C5B-O5B
3	2-I	4759[C]	FAD	O4B-C4B-C5B-O5B
4	1-J	4759[A]	FAD	O4B-C4B-C5B-O5B
3	2-O	4750[C]	FAD	O4B-C4B-C5B-O5B
3	2-C	4753[C]	FAD	O4'-C4'-C5'-O5'
3	1-D	4753[A]	FAD	O4'-C4'-C5'-O5'

There are no ring outliers.

20 monomers are involved in 154 short contacts:

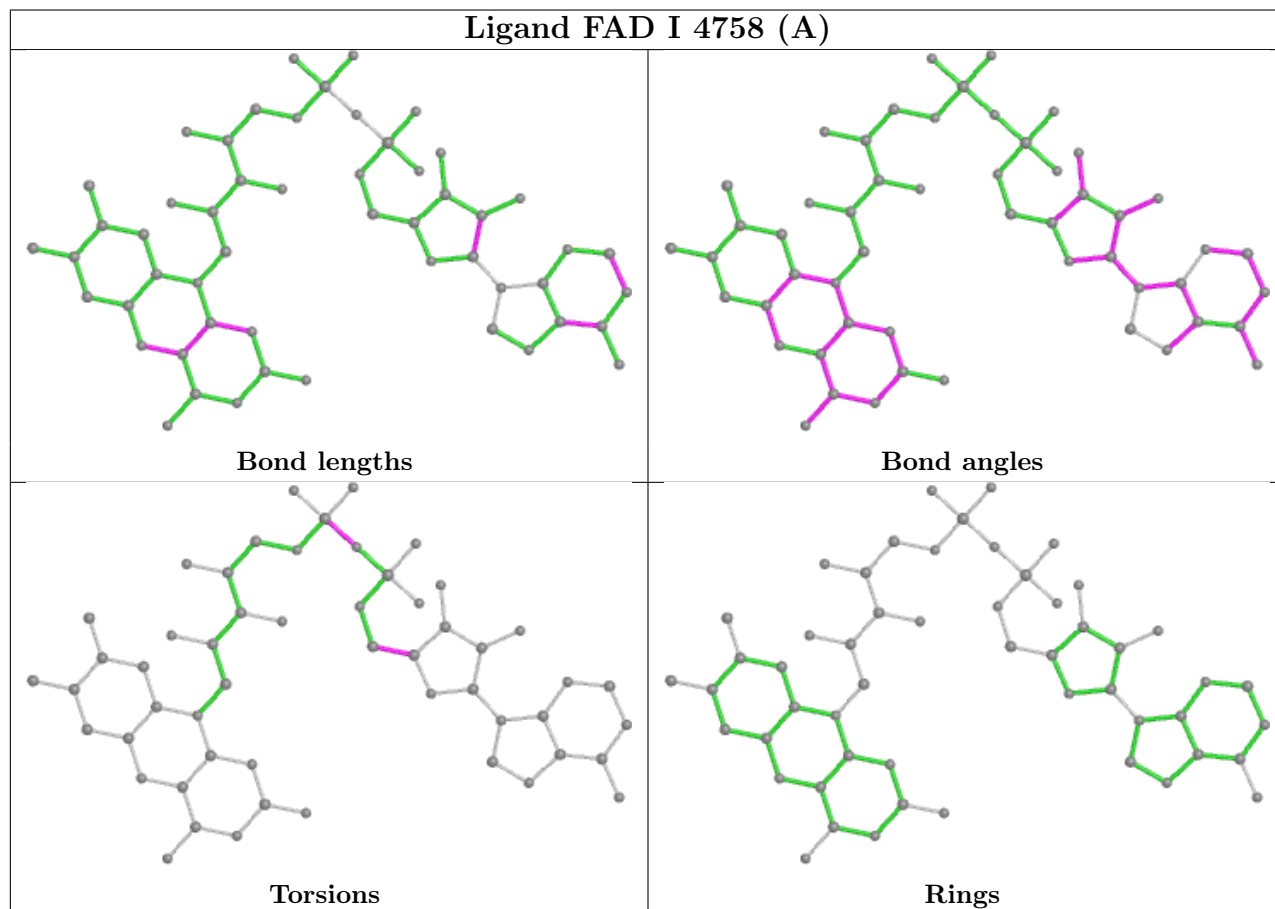
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	1-I	4758[A]	FAD	9	0
3	2-A	4751[C]	FAD	11	0
3	2-I	4759[C]	FAD	17	0
3	1-G	4756[A]	FAD	2	0
3	2-D	4754[C]	FAD	4	0
3	2-G	4757[C]	FAD	4	0
3	2-C	4753[C]	FAD	5	0
3	1-F	4755[A]	FAD	10	0
4	1-J	4759[A]	FAD	17	0
3	2-E	4755[C]	FAD	10	0
3	1-E	4754[A]	FAD	4	0
3	2-B	4752[C]	FAD	7	0
3	1-A	4750[A]	FAD	8	0
3	1-B	4751[A]	FAD	11	0
3	2-F	4756[C]	FAD	2	0

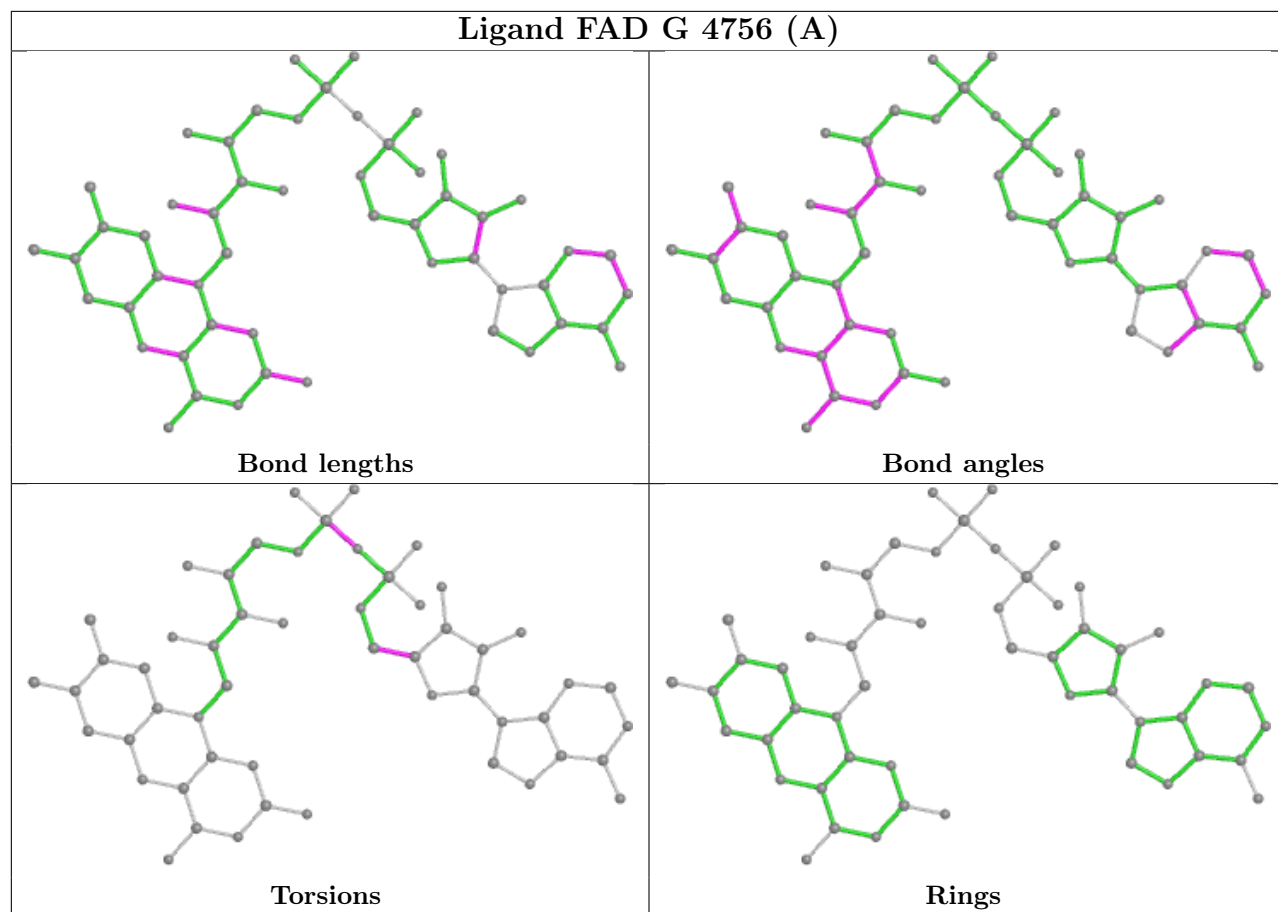
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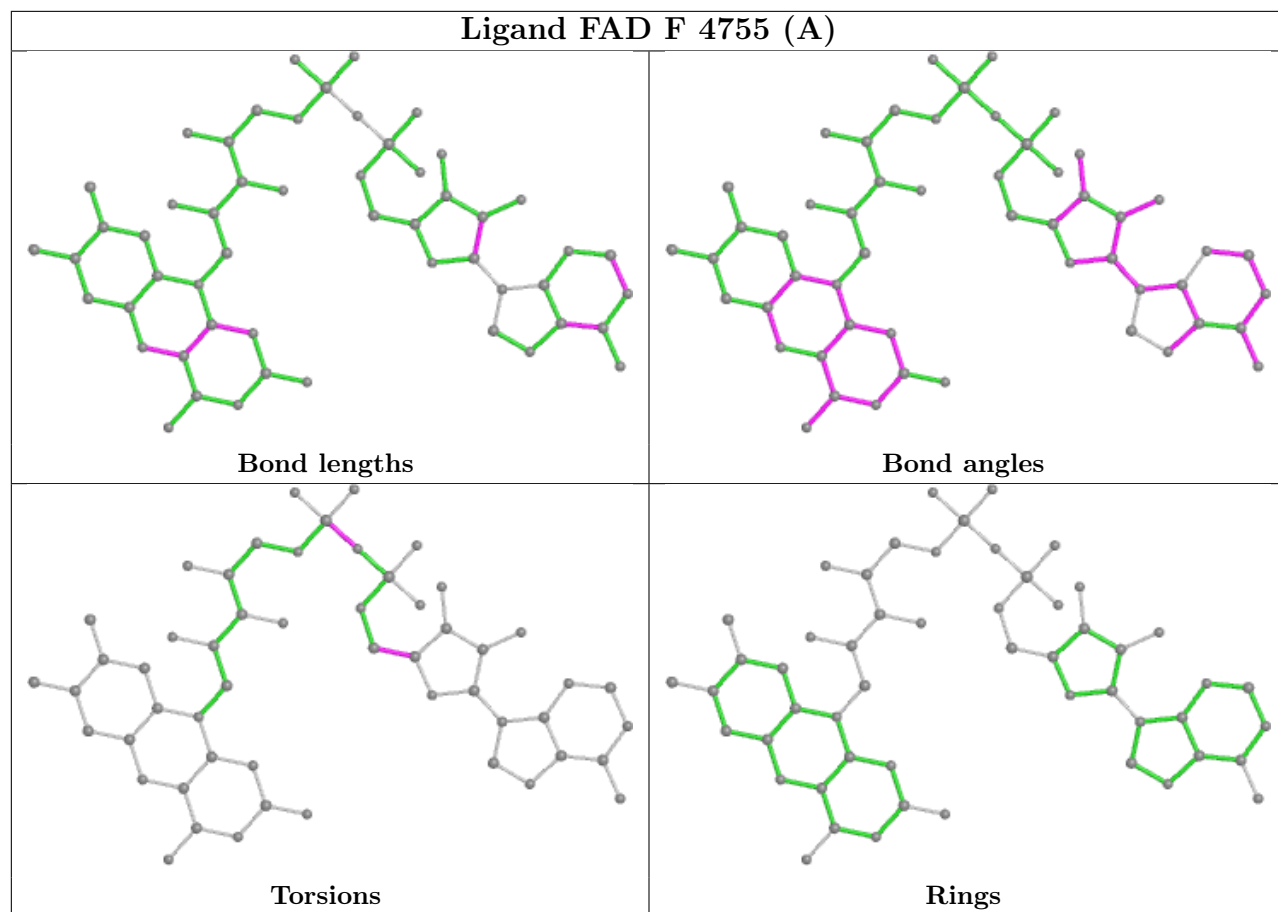
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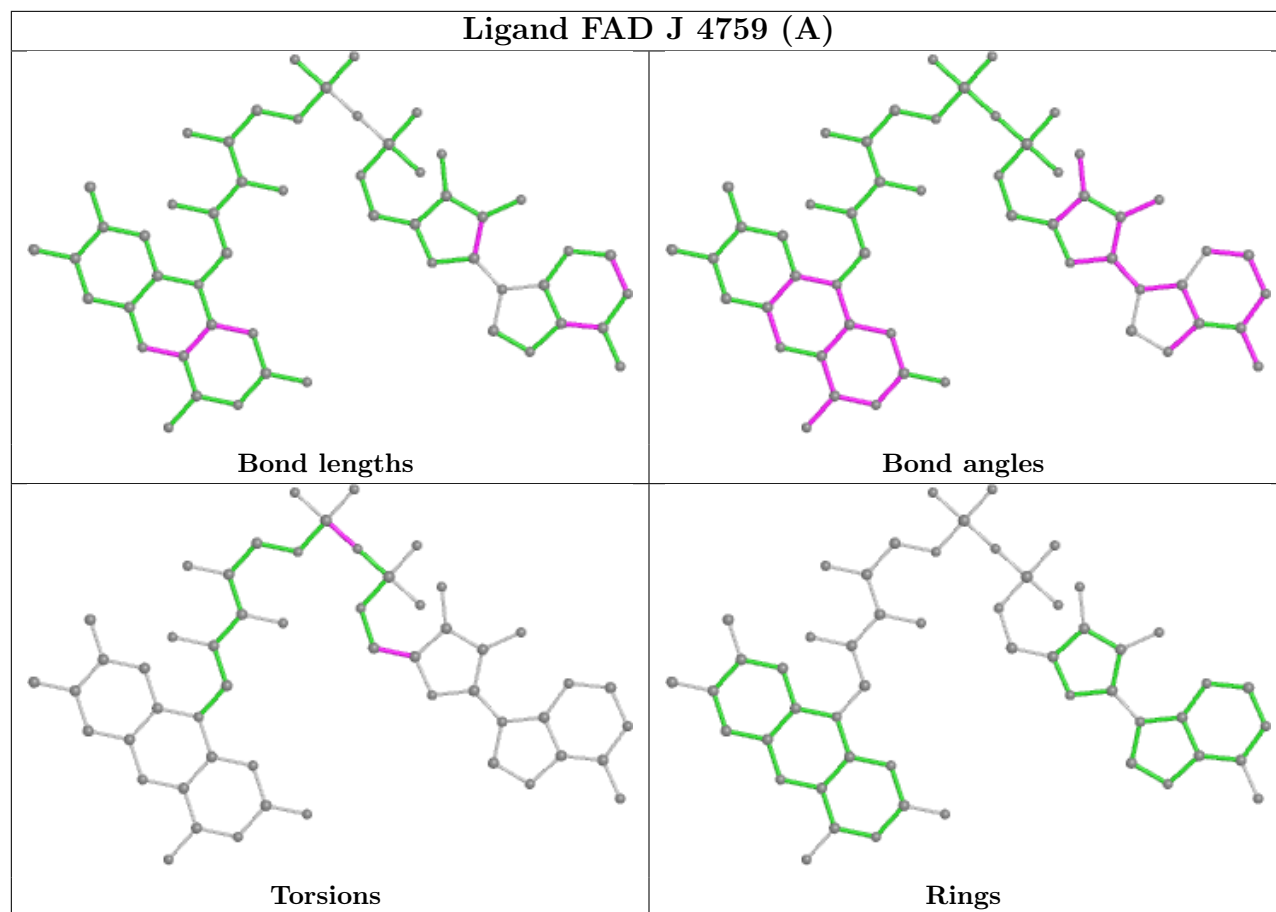
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	1-H	4757[A]	FAD	4	0
3	2-O	4750[C]	FAD	8	0
3	1-C	4752[A]	FAD	7	0
3	1-D	4753[A]	FAD	5	0
3	2-H	4758[C]	FAD	9	0

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.

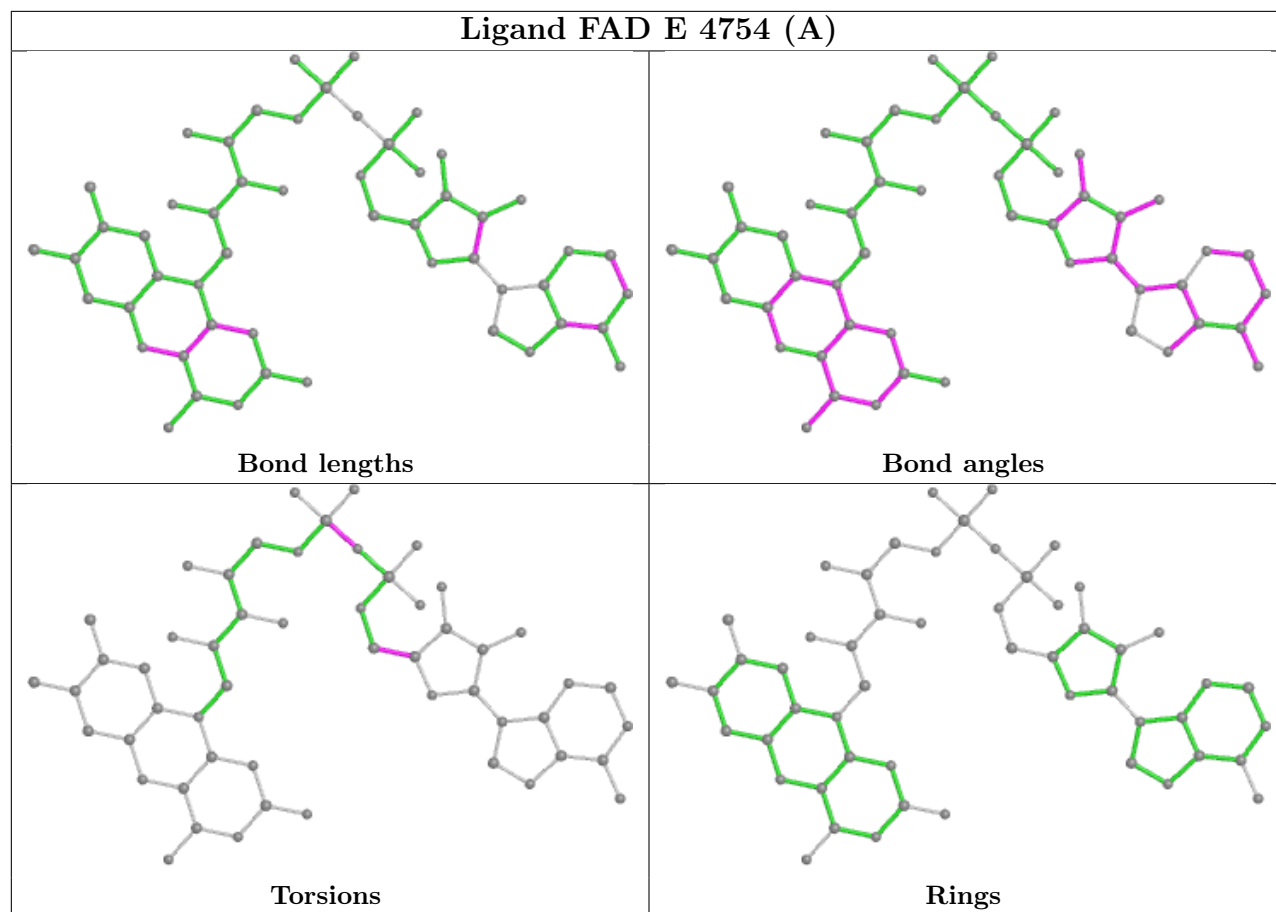


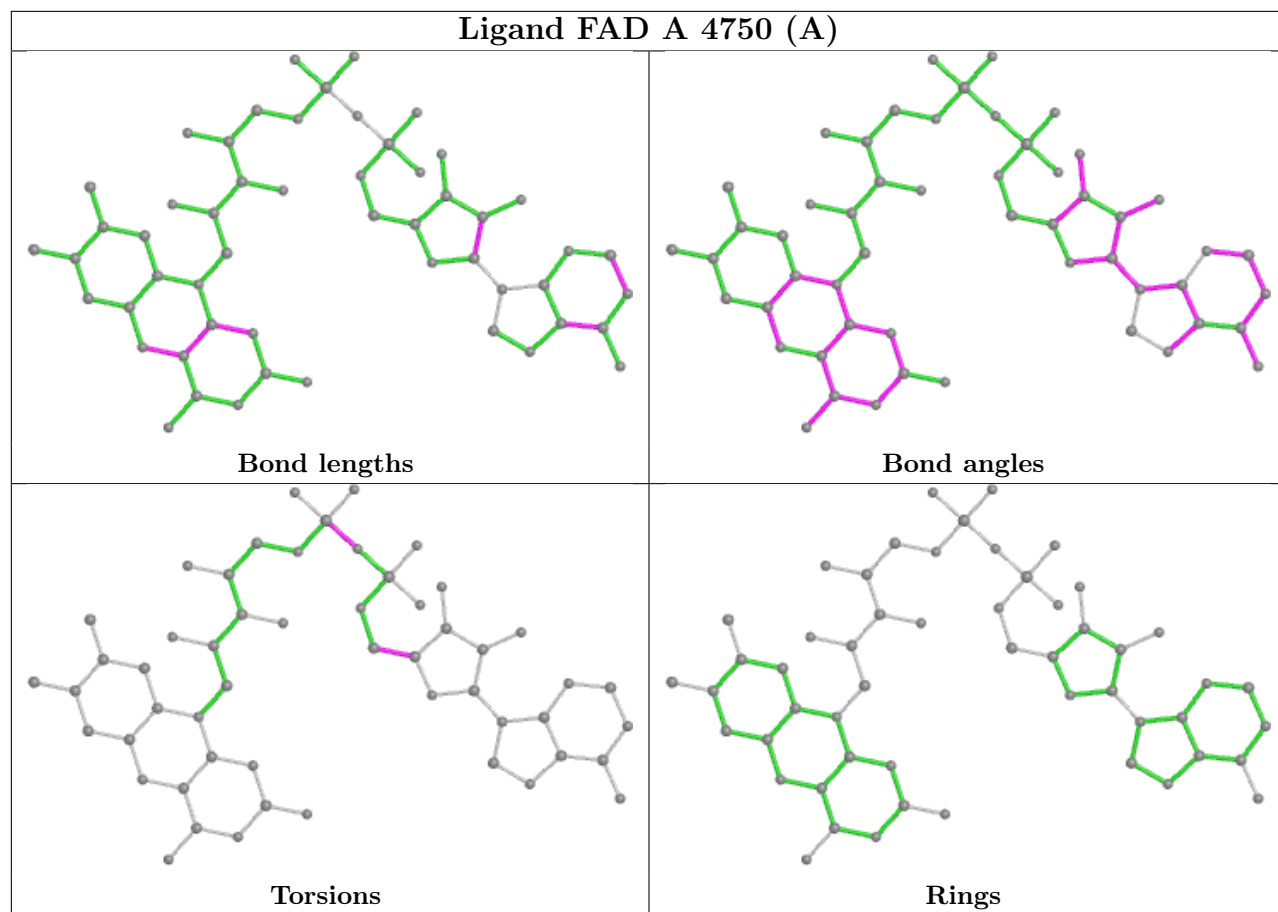


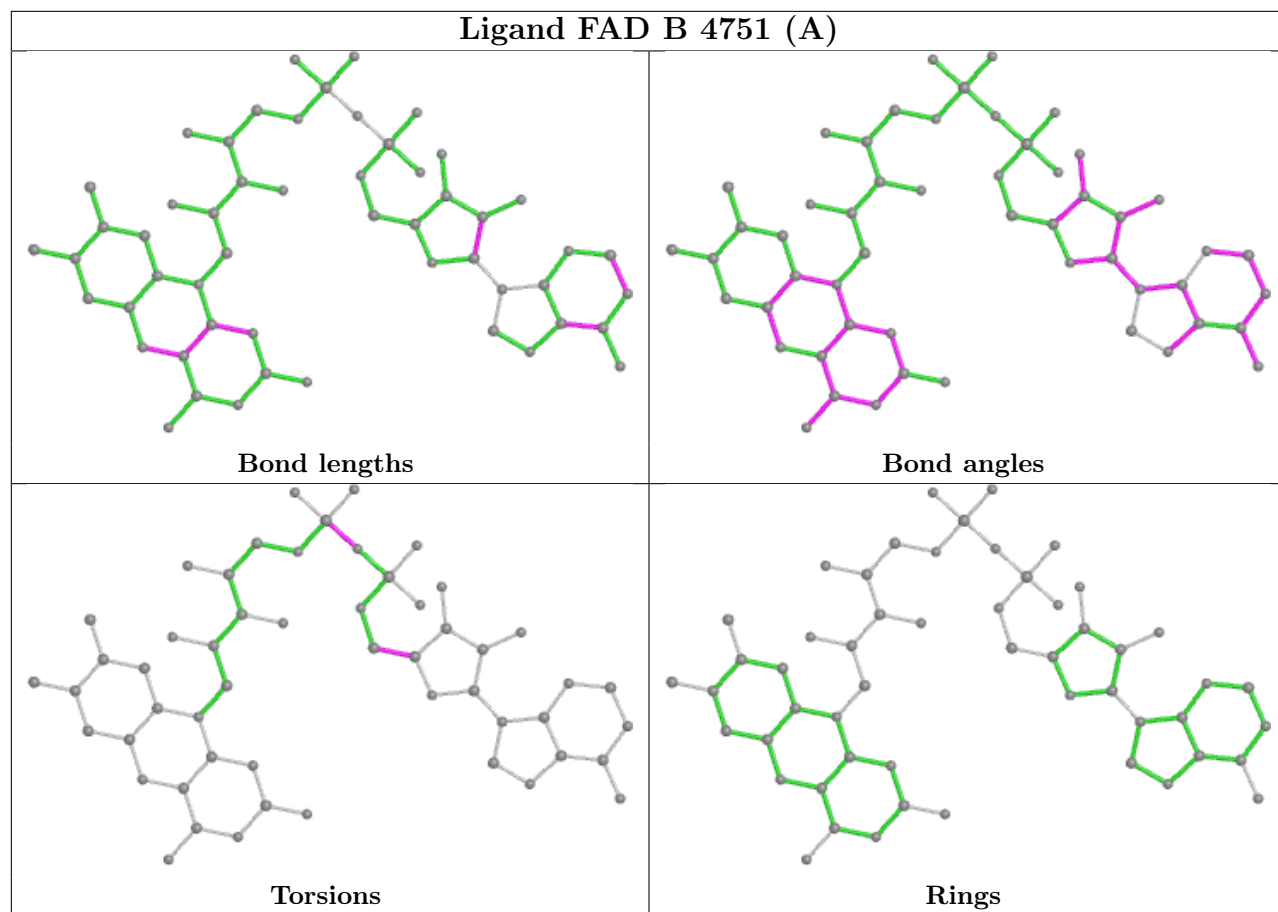


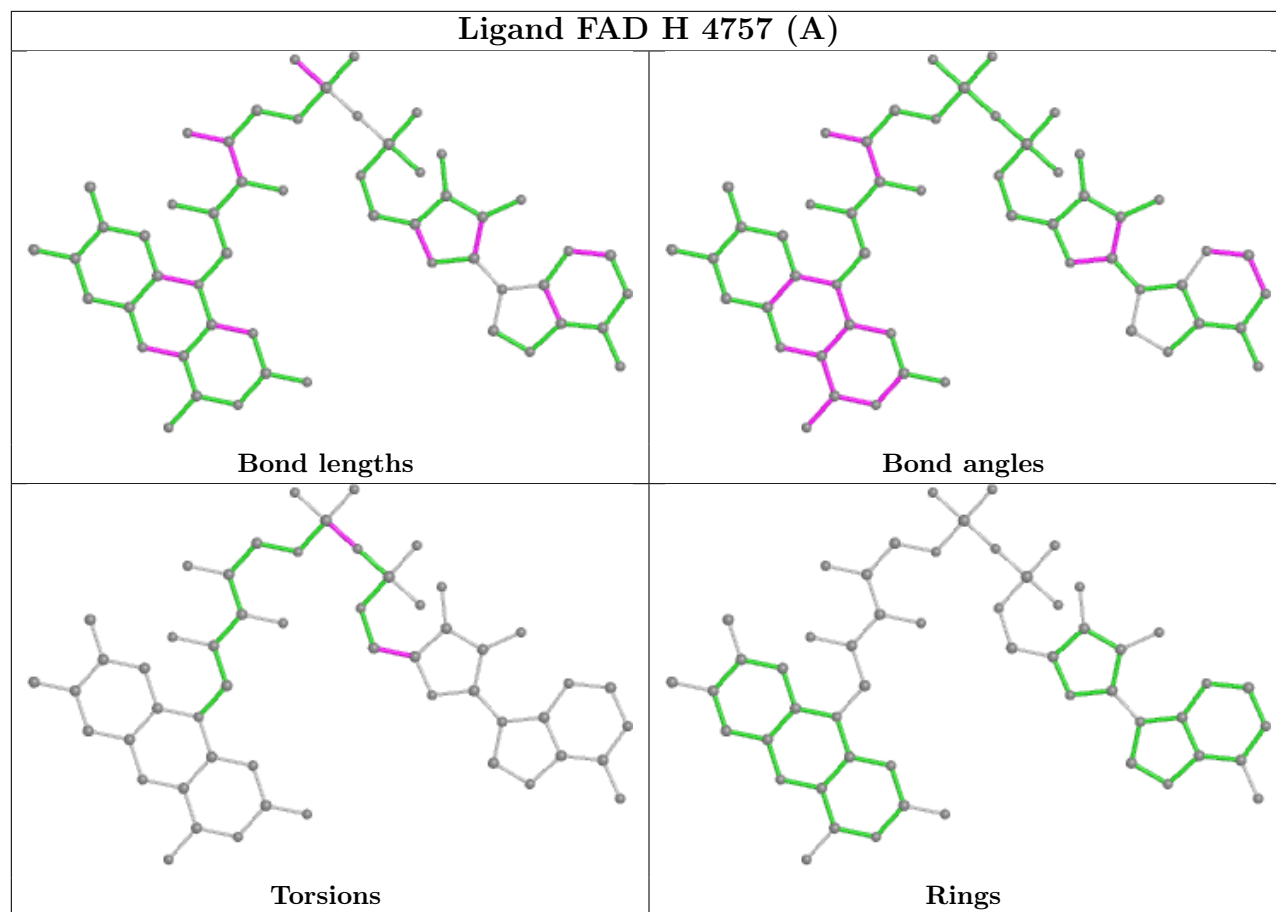


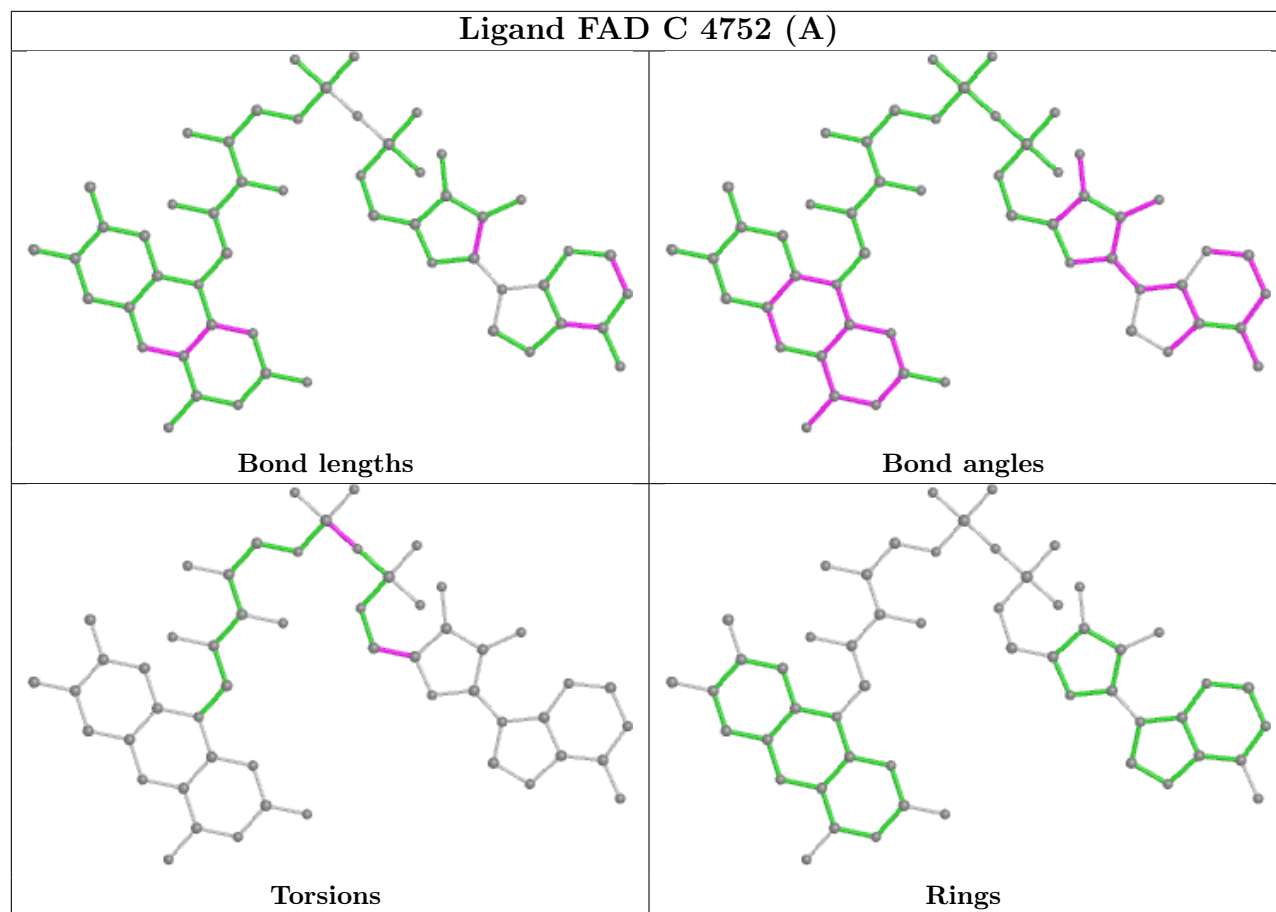


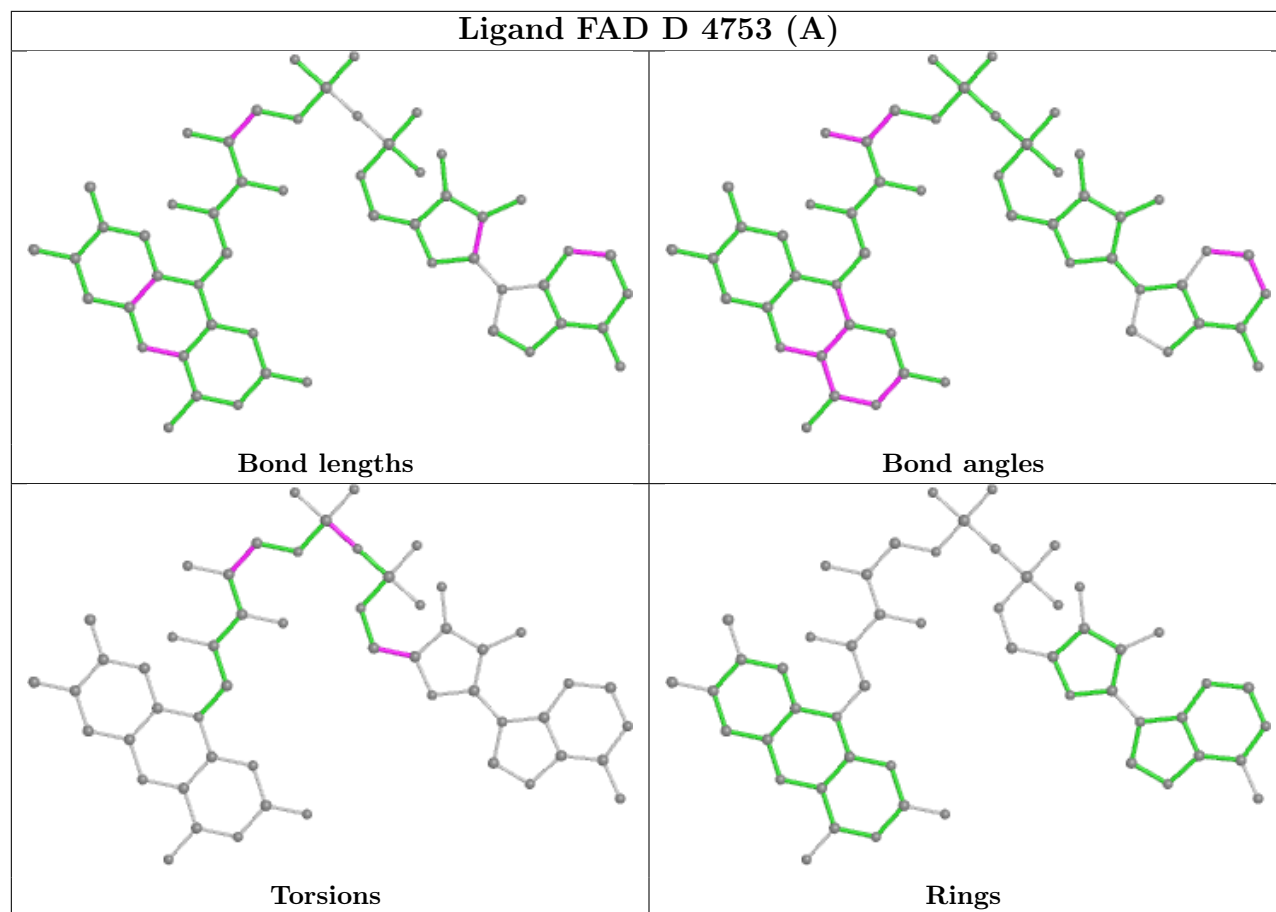












#### 4.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 5 Fit of model and data

### 5.1 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	1-A	474/474 (100%)	-0.13	5 (1%) 80 78	16, 34, 60, 86	474 (100%)
1	1-B	474/474 (100%)	-0.18	5 (1%) 80 78	15, 30, 51, 84	474 (100%)
1	1-C	474/474 (100%)	-0.30	2 (0%) 92 91	10, 24, 42, 92	474 (100%)
1	1-D	474/474 (100%)	-0.20	4 (0%) 86 84	15, 31, 54, 97	474 (100%)
1	1-E	474/474 (100%)	-0.20	1 (0%) 95 95	10, 27, 47, 94	474 (100%)
1	1-F	474/474 (100%)	-0.16	6 (1%) 77 73	15, 31, 53, 91	474 (100%)
1	1-G	474/474 (100%)	0.01	8 (1%) 70 66	16, 37, 63, 85	474 (100%)
1	1-H	474/474 (100%)	-0.33	0 100 100	10, 27, 46, 71	474 (100%)
1	1-I	474/474 (100%)	0.53	37 (7%) 13 9	18, 55, 92, 105	474 (100%)
1	1-J	474/474 (100%)	0.13	12 (2%) 57 51	20, 47, 73, 93	474 (100%)
1	2-A	474/474 (100%)	-0.13	5 (1%) 80 78	16, 34, 60, 86	474 (100%)
1	2-B	474/474 (100%)	-0.18	5 (1%) 80 78	15, 30, 51, 84	474 (100%)
1	2-C	474/474 (100%)	-0.30	2 (0%) 92 91	10, 24, 42, 92	474 (100%)
1	2-D	474/474 (100%)	-0.20	4 (0%) 86 84	15, 31, 54, 97	474 (100%)
1	2-E	474/474 (100%)	-0.20	1 (0%) 95 95	10, 27, 47, 94	474 (100%)
1	2-F	474/474 (100%)	-0.16	6 (1%) 77 73	15, 31, 53, 91	474 (100%)
1	2-G	474/474 (100%)	0.01	8 (1%) 70 66	16, 37, 63, 85	474 (100%)
1	2-H	474/474 (100%)	-0.33	0 100 100	10, 27, 46, 71	474 (100%)
1	2-I	474/474 (100%)	0.53	37 (7%) 13 9	18, 55, 92, 105	474 (100%)
1	2-J	474/474 (100%)	0.13	12 (2%) 57 51	20, 47, 73, 93	474 (100%)
2	1-K	44/229 (19%)	2.63	28 (63%) 0 0	38, 52, 59, 63	44 (100%)
2	1-L	44/229 (19%)	1.70	13 (29%) 0 0	30, 43, 53, 62	44 (100%)
2	1-M	44/229 (19%)	1.69	12 (27%) 0 0	17, 39, 54, 62	44 (100%)
2	1-N	44/229 (19%)	2.40	25 (56%) 0 0	25, 44, 57, 62	44 (100%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
2	1-O	44/229 (19%)	1.93	18 (40%) 0 0	43, 61, 74, 79	44 (100%)
2	2-K	42/229 (18%)	2.60	26 (61%) 0 0	38, 52, 59, 63	42 (100%)
2	2-L	42/229 (18%)	1.69	12 (28%) 0 0	30, 43, 51, 55	42 (100%)
2	2-M	43/229 (18%)	1.66	11 (25%) 0 0	17, 39, 52, 60	43 (100%)
2	2-N	42/229 (18%)	2.37	23 (54%) 0 0	25, 44, 57, 62	42 (100%)
All	All	9869/11541 (85%)	0.00	328 (3%) 51 39	10, 33, 67, 105	9869 (100%)

All (328) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1-E	1[A]	ALA	9.0
1	2-E	1[C]	ALA	9.0
1	1-D	1[A]	ALA	7.4
1	2-D	1[C]	ALA	7.4
1	1-C	1[A]	ALA	6.8
1	2-C	1[C]	ALA	6.8
2	1-N	171[A]	GLN	6.8
2	2-N	171[C]	GLN	6.8
2	1-M	150[A]	THR	6.7
2	2-M	150[C]	THR	6.7
2	1-K	169[A]	LEU	6.7
2	2-K	169[C]	LEU	6.7
2	1-K	171[A]	GLN	6.6
2	2-K	171[C]	GLN	6.6
1	1-J	1[A]	ALA	6.5
1	2-J	1[C]	ALA	6.5
2	1-O	149[A]	GLY	6.2
2	1-N	167[A]	VAL	5.9
2	2-N	167[C]	VAL	5.9
2	1-M	171[A]	GLN	5.7
2	2-M	171[C]	GLN	5.7
2	1-L	150[A]	THR	5.6
2	2-L	150[C]	THR	5.6
2	1-O	150[A]	THR	5.6
1	1-I	1[A]	ALA	5.6
1	2-I	1[C]	ALA	5.6
2	1-O	151[A]	ALA	5.6
2	1-L	171[A]	GLN	5.5
2	2-L	171[C]	GLN	5.5
2	1-N	170[A]	LYS	5.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	2-N	170[C]	LYS	5.5
2	1-N	148[A]	GLN	5.5
2	2-N	148[C]	GLN	5.5
2	1-L	169[A]	LEU	5.4
2	2-L	169[C]	LEU	5.4
2	1-M	172[A]	THR	5.1
2	2-M	172[C]	THR	5.1
1	1-J	468[A]	PHE	4.9
1	2-J	468[C]	PHE	4.9
2	1-N	143[A]	SER	4.8
2	2-N	143[C]	SER	4.8
2	1-N	150[A]	THR	4.8
2	2-N	150[C]	THR	4.8
2	1-N	145[A]	ASP	4.7
2	2-N	145[C]	ASP	4.7
2	1-K	163[A]	ALA	4.7
2	2-K	163[C]	ALA	4.7
2	1-N	147[A]	SER	4.6
2	2-N	147[C]	SER	4.6
2	1-K	148[A]	GLN	4.5
2	2-K	148[C]	GLN	4.5
2	1-K	144[A]	LEU	4.4
2	2-K	144[C]	LEU	4.4
2	1-K	133[A]	PRO	4.4
2	2-K	133[C]	PRO	4.4
2	1-O	168[A]	GLN	4.3
2	1-K	168[A]	GLN	4.3
2	2-K	168[C]	GLN	4.3
2	1-M	167[A]	VAL	4.2
2	2-M	167[C]	VAL	4.2
2	1-L	162[A]	ASP	4.2
2	2-L	162[C]	ASP	4.2
2	1-N	133[A]	PRO	4.2
2	2-N	133[C]	PRO	4.2
2	1-K	141[A]	LYS	4.2
2	2-K	141[C]	LYS	4.2
1	1-G	1[A]	ALA	4.1
1	2-G	1[C]	ALA	4.1
2	1-M	166[A]	LEU	4.1
2	2-M	166[C]	LEU	4.1
2	1-L	165[A]	LYS	4.1
2	2-L	165[C]	LYS	4.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	1-K	136[A]	ARG	4.0
2	2-K	136[C]	ARG	4.0
2	1-K	147[A]	SER	4.0
2	2-K	147[C]	SER	4.0
1	1-D	134[A]	GLY	4.0
1	2-D	134[C]	GLY	4.0
2	1-N	149[A]	GLY	3.9
2	2-N	149[C]	GLY	3.9
2	1-O	158[A]	PHE	3.8
2	1-K	139[A]	LEU	3.8
2	1-O	139[A]	LEU	3.8
2	2-K	139[C]	LEU	3.8
1	1-I	294[A]	ILE	3.8
1	2-I	294[C]	ILE	3.8
2	1-K	161[A]	GLU	3.8
2	2-K	161[C]	GLU	3.8
2	1-M	145[A]	ASP	3.7
2	2-M	145[C]	ASP	3.7
2	1-K	151[A]	ALA	3.7
2	2-K	151[C]	ALA	3.7
2	1-K	170[A]	LYS	3.7
2	2-K	170[C]	LYS	3.7
1	1-G	132[A]	ALA	3.7
1	2-G	132[C]	ALA	3.7
1	1-I	121[A]	ILE	3.7
1	2-I	121[C]	ILE	3.7
2	1-O	171[A]	GLN	3.7
2	1-N	169[A]	LEU	3.6
2	2-N	169[C]	LEU	3.6
2	1-K	167[A]	VAL	3.6
2	2-K	167[C]	VAL	3.6
2	1-N	146[A]	ALA	3.6
2	2-N	146[C]	ALA	3.6
2	1-N	161[A]	GLU	3.6
2	2-N	161[C]	GLU	3.6
2	1-K	135[A]	ALA	3.5
2	2-K	135[C]	ALA	3.5
2	1-M	147[A]	SER	3.5
2	2-M	147[C]	SER	3.5
2	1-L	170[A]	LYS	3.5
2	2-L	170[C]	LYS	3.5
1	1-I	136[A]	THR	3.5

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Mol	Chain	Res	Type	RSRZ
1	2-I	136[C]	THR	3.5
1	1-I	303[A]	PRO	3.5
1	2-I	303[C]	PRO	3.5
2	1-M	168[A]	GLN	3.4
2	2-M	168[C]	GLN	3.4
2	1-K	172[A]	THR	3.3
1	1-I	287[A]	LEU	3.3
1	2-I	287[C]	LEU	3.3
2	1-N	144[A]	LEU	3.3
2	2-N	144[C]	LEU	3.3
2	1-K	150[A]	THR	3.3
2	2-K	150[C]	THR	3.3
2	1-K	146[A]	ALA	3.3
2	2-K	146[C]	ALA	3.3
1	1-I	135[A]	GLY	3.2
1	2-I	135[C]	GLY	3.2
1	1-I	33[A]	VAL	3.2
1	2-I	33[C]	VAL	3.2
2	1-N	173[A]	GLY	3.2
2	1-N	168[A]	GLN	3.1
2	2-N	168[C]	GLN	3.1
2	1-O	163[A]	ALA	3.1
1	1-A	79[A]	SER	3.1
1	2-A	79[C]	SER	3.1
1	1-F	1[A]	ALA	3.1
1	1-I	138[A]	VAL	3.1
1	2-F	1[C]	ALA	3.1
1	2-I	138[C]	VAL	3.1
2	1-K	143[A]	SER	3.1
2	2-K	143[C]	SER	3.1
2	1-M	163[A]	ALA	3.1
2	2-M	163[C]	ALA	3.1
2	1-K	142[A]	HIS	3.0
2	2-K	142[C]	HIS	3.0
1	1-B	1[A]	ALA	3.0
1	2-B	1[C]	ALA	3.0
2	1-N	172[A]	THR	3.0
2	1-O	131[A]	LEU	3.0
1	1-I	144[A]	ILE	3.0
1	2-I	144[C]	ILE	3.0
2	1-O	166[A]	LEU	3.0
1	1-I	263[A]	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	2-I	263[C]	GLY	3.0
2	1-L	173[A]	GLY	3.0
2	1-K	164[A]	LEU	2.9
2	2-K	164[C]	LEU	2.9
1	1-D	132[A]	ALA	2.9
1	2-D	132[C]	ALA	2.9
1	1-I	146[A]	ILE	2.9
1	2-I	146[C]	ILE	2.9
2	1-K	173[A]	GLY	2.9
2	1-K	138[A]	ILE	2.9
2	2-K	138[C]	ILE	2.9
2	1-N	134[A]	ALA	2.8
2	2-N	134[C]	ALA	2.8
1	1-F	262[A]	SER	2.8
1	2-F	262[C]	SER	2.8
1	1-A	1[A]	ALA	2.8
1	2-A	1[C]	ALA	2.8
2	1-O	144[A]	LEU	2.8
2	1-O	165[A]	LYS	2.8
1	1-G	207[A]	VAL	2.7
1	2-G	207[C]	VAL	2.7
1	1-J	470[A]	LYS	2.7
1	2-J	470[C]	LYS	2.7
1	1-I	4[A]	PRO	2.7
1	2-I	4[C]	PRO	2.7
2	1-M	170[A]	LYS	2.7
2	2-M	170[C]	LYS	2.7
1	1-F	132[A]	ALA	2.7
1	2-F	132[C]	ALA	2.7
1	1-I	133[A]	ASP	2.7
1	2-I	133[C]	ASP	2.7
2	1-M	173[A]	GLY	2.7
2	1-O	147[A]	SER	2.6
1	1-G	266[A]	ALA	2.6
1	2-G	266[C]	ALA	2.6
2	1-N	166[A]	LEU	2.6
2	2-N	166[C]	LEU	2.6
1	1-C	2[A]	ASP	2.6
1	2-C	2[C]	ASP	2.6
1	1-I	295[A]	GLU	2.6
1	2-I	295[C]	GLU	2.6
2	1-K	134[A]	ALA	2.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	2-K	134[C]	ALA	2.6
1	1-I	30[A]	PHE	2.5
1	2-I	30[C]	PHE	2.5
1	1-I	10[A]	THR	2.5
1	1-I	316[A]	TYR	2.5
1	2-I	10[C]	THR	2.5
1	2-I	316[C]	TYR	2.5
2	1-M	161[A]	GLU	2.5
2	2-M	161[C]	GLU	2.5
1	1-F	2[A]	ASP	2.5
1	2-F	2[C]	ASP	2.5
2	1-N	164[A]	LEU	2.5
2	2-N	164[C]	LEU	2.5
1	1-I	379[A]	ILE	2.5
1	2-I	379[C]	ILE	2.5
1	1-J	456[A]	SER	2.5
1	2-J	456[C]	SER	2.5
1	1-J	413[A]	ASP	2.5
1	2-J	413[C]	ASP	2.5
2	1-N	163[A]	ALA	2.5
2	2-N	163[C]	ALA	2.5
1	1-J	39[A]	GLU	2.5
1	2-J	39[C]	GLU	2.5
1	1-I	315[A]	ILE	2.5
1	2-I	315[C]	ILE	2.5
2	1-L	149[A]	GLY	2.5
2	2-L	149[C]	GLY	2.5
1	1-I	292[A]	LEU	2.4
1	2-I	292[C]	LEU	2.4
1	1-I	31[A]	LYS	2.4
1	2-I	31[C]	LYS	2.4
1	1-I	79[A]	SER	2.4
1	2-I	79[C]	SER	2.4
2	1-L	161[A]	GLU	2.4
2	2-L	161[C]	GLU	2.4
1	1-A	265[A]	LYS	2.4
1	2-A	265[C]	LYS	2.4
1	1-I	6[A]	ASP	2.4
1	2-I	6[C]	ASP	2.4
2	1-O	148[A]	GLN	2.4
1	1-G	258[A]	ILE	2.4
1	2-G	258[C]	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	1-I	5[A]	ILE	2.4
1	2-I	5[C]	ILE	2.4
2	1-N	135[A]	ALA	2.4
2	2-N	135[C]	ALA	2.4
1	1-I	111[A]	LYS	2.3
1	2-I	111[C]	LYS	2.3
1	1-J	135[A]	GLY	2.3
1	2-J	135[C]	GLY	2.3
1	1-F	82[A]	ARG	2.3
1	2-F	82[C]	ARG	2.3
2	1-L	146[A]	ALA	2.3
2	2-L	146[C]	ALA	2.3
1	1-D	136[A]	THR	2.3
1	2-D	136[C]	THR	2.3
2	1-L	168[A]	GLN	2.3
2	2-L	168[C]	GLN	2.3
1	1-I	468[A]	PHE	2.2
1	2-I	468[C]	PHE	2.2
1	1-I	2[A]	ASP	2.2
1	2-I	2[C]	ASP	2.2
2	1-K	145[A]	ASP	2.2
2	2-K	145[C]	ASP	2.2
1	1-B	79[A]	SER	2.2
1	2-B	79[C]	SER	2.2
2	1-O	146[A]	ALA	2.2
1	1-J	4[A]	PRO	2.2
1	2-J	4[C]	PRO	2.2
2	1-N	136[A]	ARG	2.2
2	2-N	136[C]	ARG	2.2
1	1-J	469[A]	GLY	2.2
1	2-J	469[C]	GLY	2.2
1	1-F	456[A]	SER	2.2
1	2-F	456[C]	SER	2.2
1	1-I	302[A]	ILE	2.1
1	2-I	302[C]	ILE	2.1
1	1-G	80[A]	GLU	2.1
1	2-G	80[C]	GLU	2.1
2	1-L	147[A]	SER	2.1
2	2-L	147[C]	SER	2.1
1	1-I	425[A]	ALA	2.1
1	1-J	311[A]	LYS	2.1
1	2-I	425[C]	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	2-J	311[C]	LYS	2.1
1	1-I	313[A]	PRO	2.1
1	2-I	313[C]	PRO	2.1
2	1-O	164[A]	LEU	2.1
1	1-B	80[A]	GLU	2.1
1	1-G	79[A]	SER	2.1
1	2-B	80[C]	GLU	2.1
1	2-G	79[C]	SER	2.1
1	1-I	113[A]	VAL	2.1
1	1-I	451[A]	ALA	2.1
1	2-I	113[C]	VAL	2.1
1	2-I	451[C]	ALA	2.1
2	1-N	151[A]	ALA	2.1
2	2-N	151[C]	ALA	2.1
1	1-A	244[A]	THR	2.1
1	2-A	244[C]	THR	2.1
1	1-J	35[A]	ILE	2.1
1	2-J	35[C]	ILE	2.1
1	1-G	358[A]	ILE	2.1
1	2-G	358[C]	ILE	2.1
1	1-B	430[A]	ASN	2.1
1	2-B	430[C]	ASN	2.1
2	1-O	161[A]	GLU	2.1
2	1-O	155[A]	ARG	2.1
1	1-I	454[A]	THR	2.0
1	2-I	454[C]	THR	2.0
2	1-N	159[A]	THR	2.0
2	2-N	159[C]	THR	2.0
1	1-J	411[A]	SER	2.0
1	2-J	411[C]	SER	2.0
2	1-L	148[A]	GLN	2.0
2	2-L	148[C]	GLN	2.0
1	1-I	311[A]	LYS	2.0
1	2-I	311[C]	LYS	2.0
1	1-I	428[A]	MET	2.0
1	2-I	428[C]	MET	2.0
2	1-K	159[A]	THR	2.0
2	2-K	159[C]	THR	2.0
1	1-A	262[A]	SER	2.0
1	1-B	356[A]	SER	2.0
1	2-A	262[C]	SER	2.0
1	2-B	356[C]	SER	2.0

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Mol	Chain	Res	Type	RSRZ
1	1-I	34[A]	CYS	2.0
1	2-I	34[C]	CYS	2.0
2	1-K	160[A]	LYS	2.0
2	2-K	160[C]	LYS	2.0

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

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

## 5.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.4 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(Å <sup>2</sup> )	Q<0.9
3	FAD	2-I	4759[C]	53/53	0.84	0.20	30,38,42,46	53
4	FAD	1-J	4759[A]	53/53	0.84	0.20	30,38,42,46	53
3	FAD	2-H	4758[C]	53/53	0.89	0.17	30,38,42,46	53
3	FAD	1-I	4758[A]	53/53	0.89	0.17	30,38,42,46	53
3	FAD	2-A	4751[C]	53/53	0.90	0.22	30,38,42,46	53
3	FAD	1-B	4751[A]	53/53	0.90	0.22	30,38,42,46	53
3	FAD	1-A	4750[A]	53/53	0.90	0.20	30,38,42,46	53
3	FAD	2-O	4750[C]	53/53	0.90	0.20	30,38,42,46	53
3	FAD	1-F	4755[A]	53/53	0.91	0.20	30,38,42,46	53
3	FAD	2-E	4755[C]	53/53	0.91	0.20	30,38,42,46	53
3	FAD	1-E	4754[A]	53/53	0.92	0.21	30,38,42,46	53
3	FAD	2-D	4754[C]	53/53	0.92	0.21	30,38,42,46	53
3	FAD	1-G	4756[A]	53/53	0.94	0.24	43,51,53,54	53
3	FAD	2-F	4756[C]	53/53	0.94	0.24	43,51,53,54	53
3	FAD	1-D	4753[A]	53/53	0.95	0.20	35,45,57,57	53
3	FAD	2-B	4752[C]	53/53	0.95	0.21	30,38,42,46	53
3	FAD	1-C	4752[A]	53/53	0.95	0.21	30,38,42,46	53
3	FAD	2-C	4753[C]	53/53	0.95	0.20	35,45,57,57	53
3	FAD	1-H	4757[A]	53/53	0.97	0.20	32,35,43,47	53

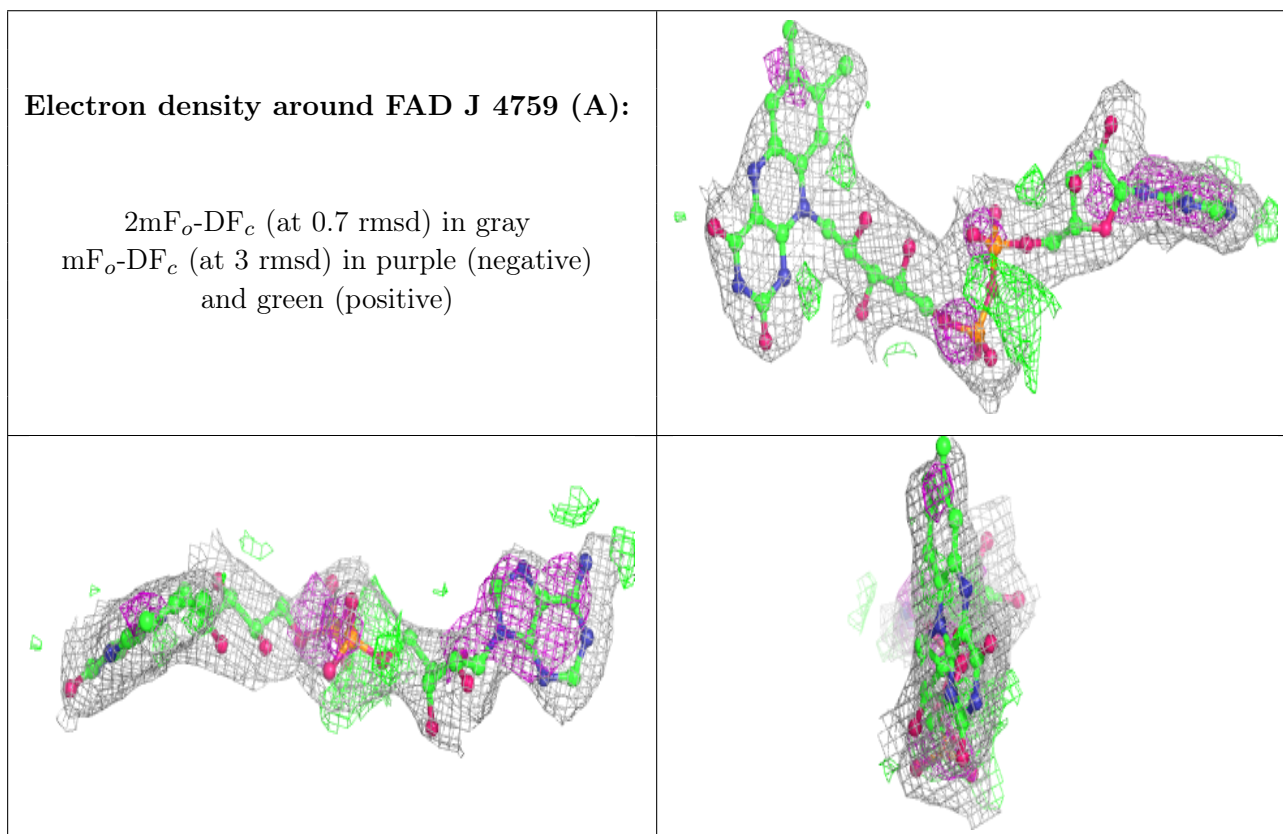
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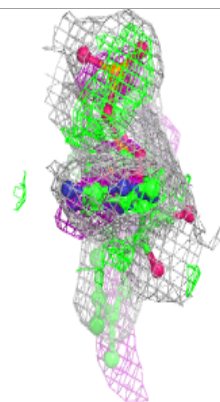
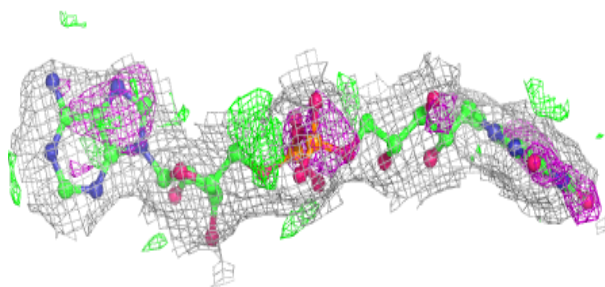
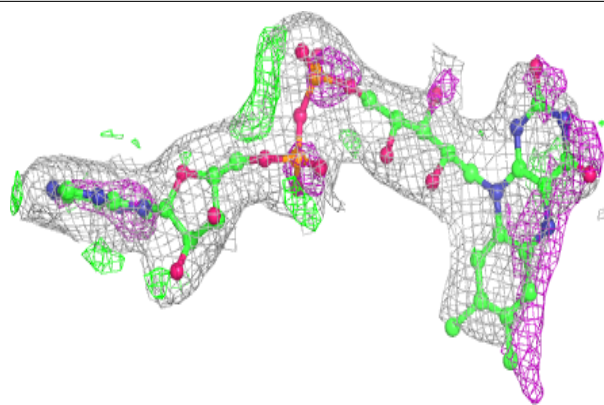
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	FAD	2-G	4757[C]	53/53	0.97	0.20	32,35,43,47	53

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.

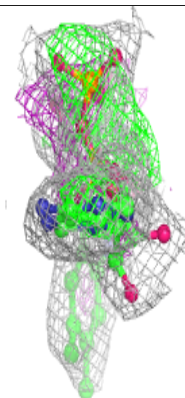
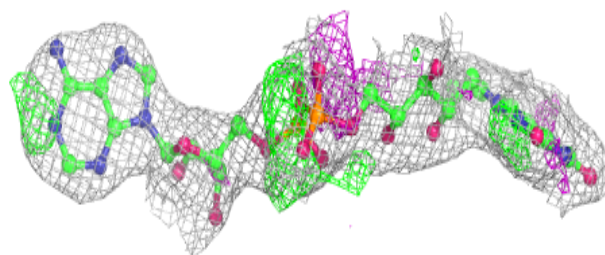
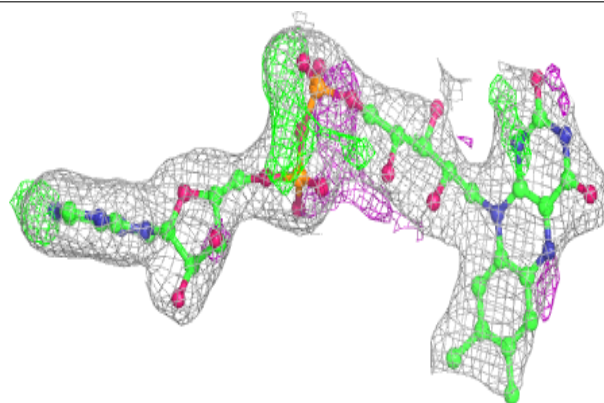


**Electron density around FAD I 4758 (A):**

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

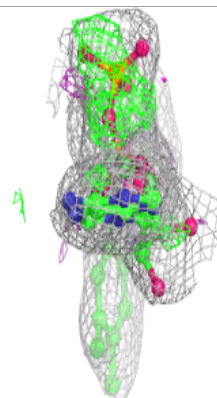
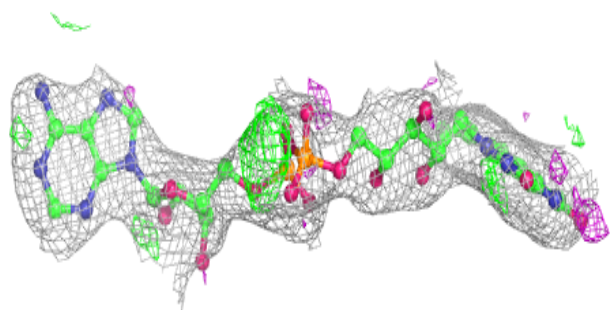
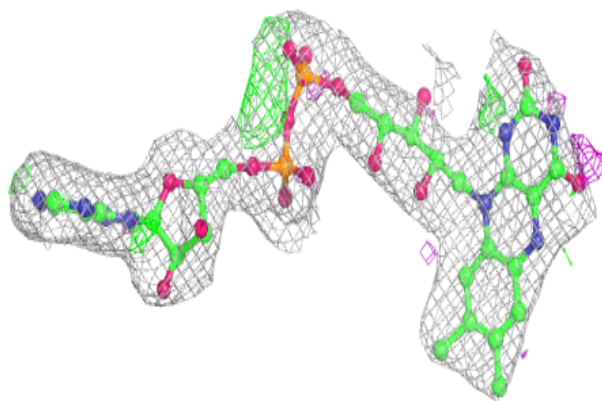
**Electron density around FAD B 4751 (A):**

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

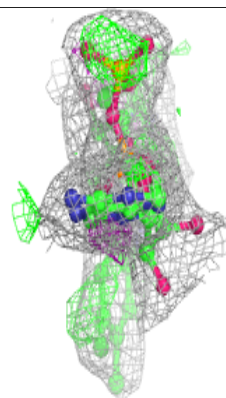
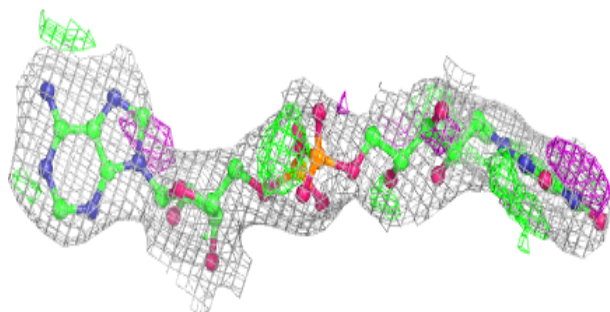
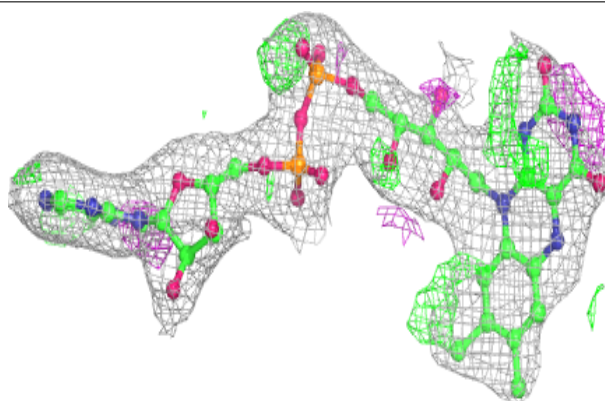


**Electron density around FAD A 4750 (A):**

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

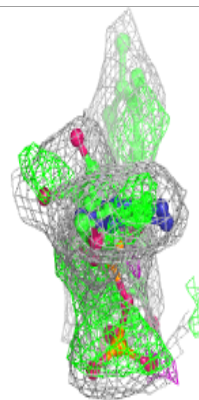
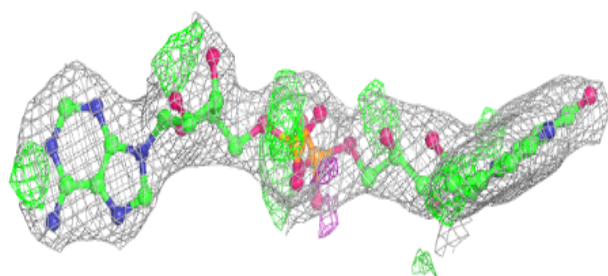
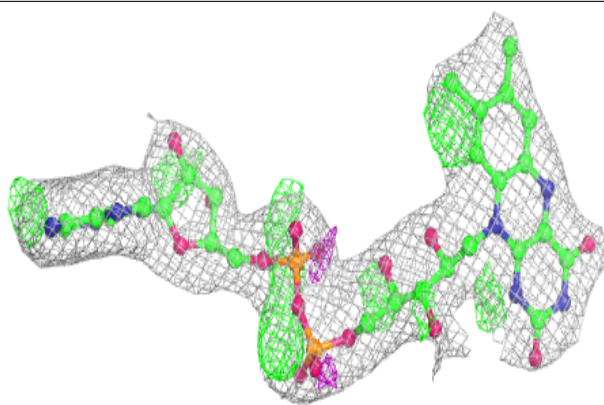
**Electron density around FAD F 4755 (A):**

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

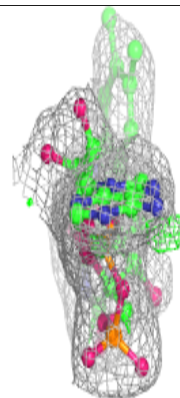
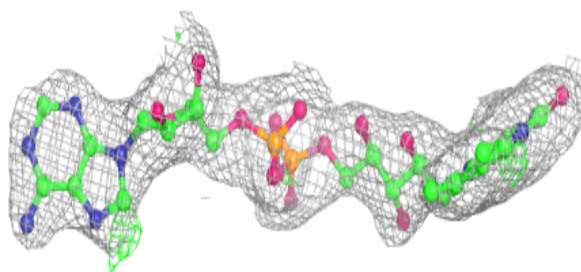
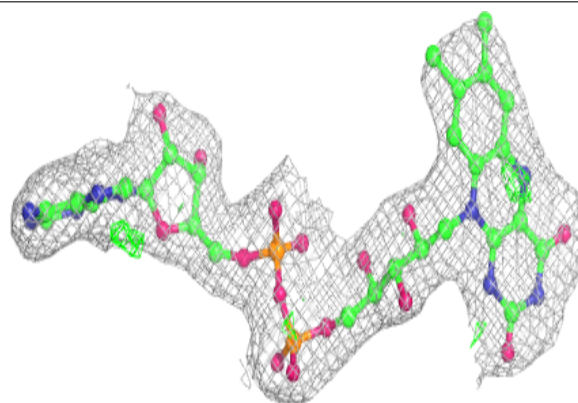


**Electron density around FAD E 4754 (A):**

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

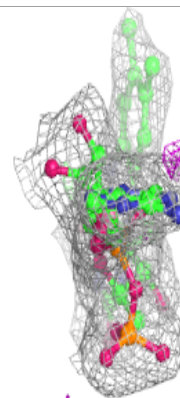
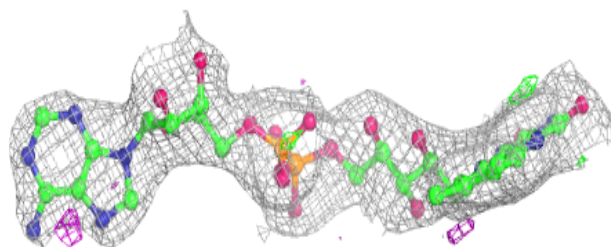
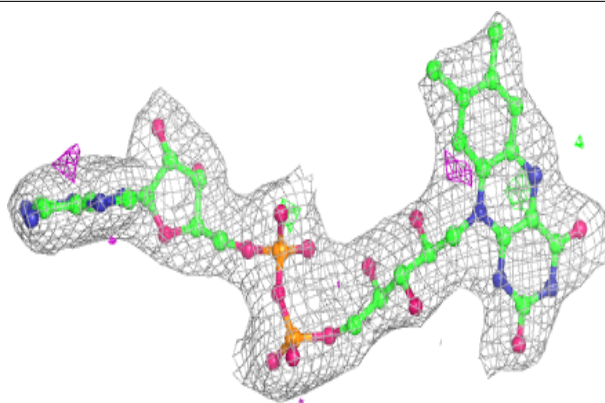
**Electron density around FAD G 4756 (A):**

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

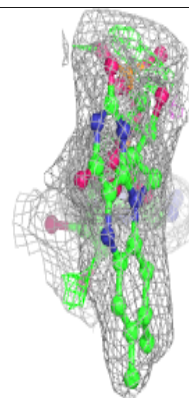
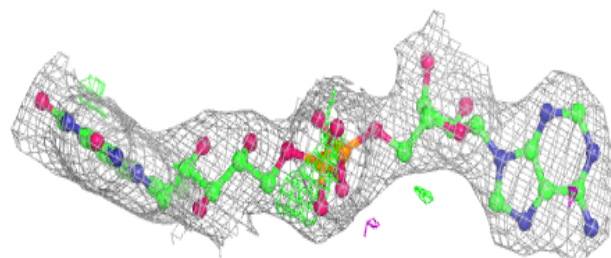
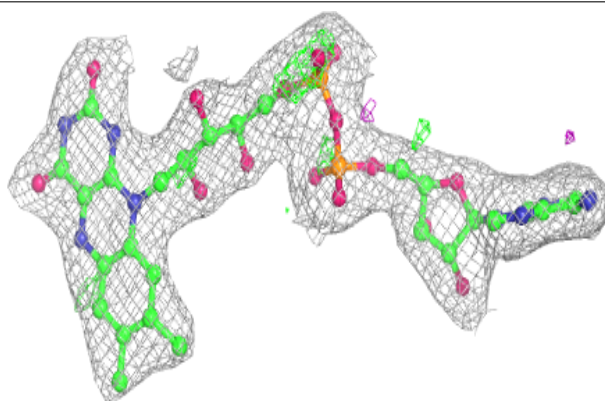


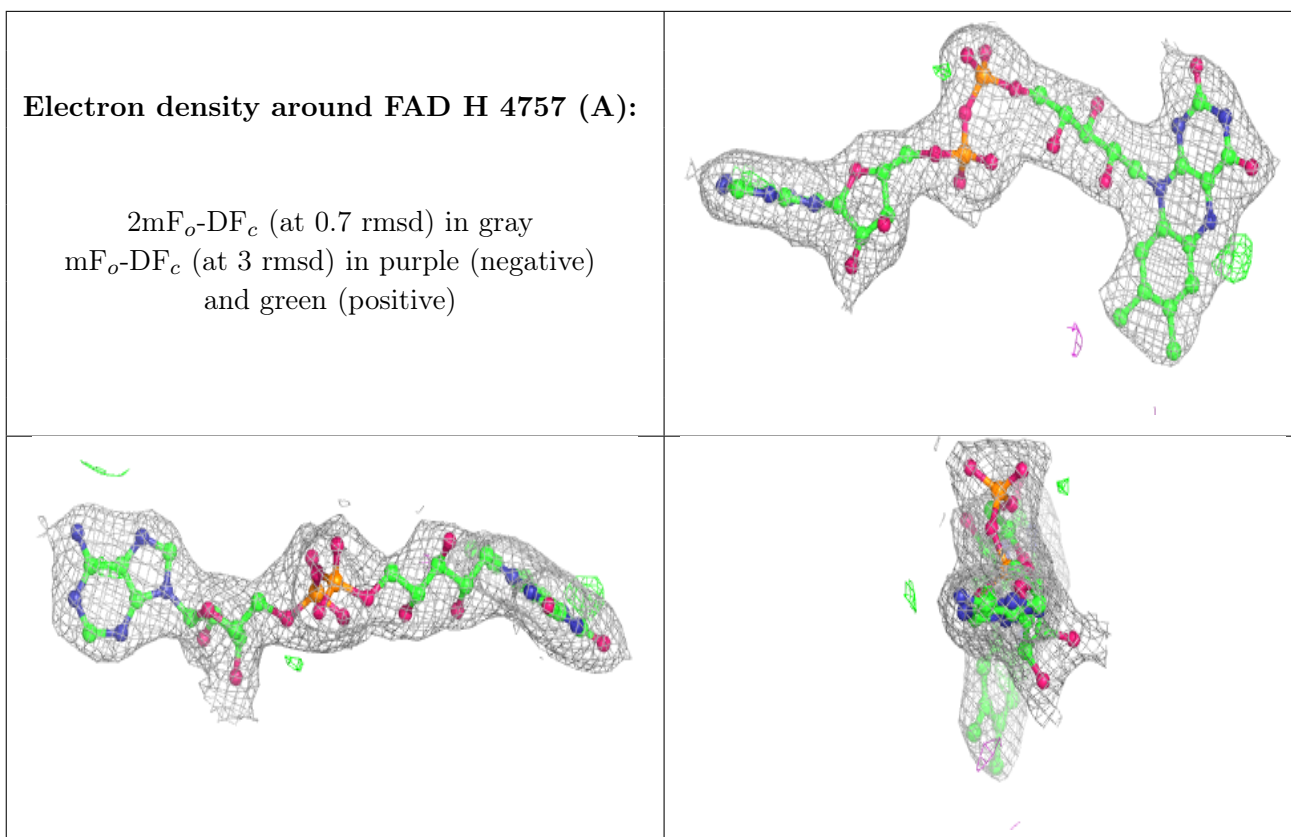
**Electron density around FAD D 4753 (A):**

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

**Electron density around FAD C 4752 (A):**

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





## 5.5 Other polymers [i](#)

There are no such residues in this entry.