Full wwPDB X-ray Structure Validation Report ⓘ

May 18, 2020 – 12:16 am BST

PDB ID	:	1PJL
Title	:	Crystal structure of human m-NAD-ME in ternary complex with NAD and Lu3+
Authors	:	Yang, Z.; Batra, R.; Floyd, D.L.; Hung, H.-C.; Chang, G.-G.; Tong, L.
Deposited on	:	2003-06-03
Resolution	:	2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ①) were used in the production of this report:

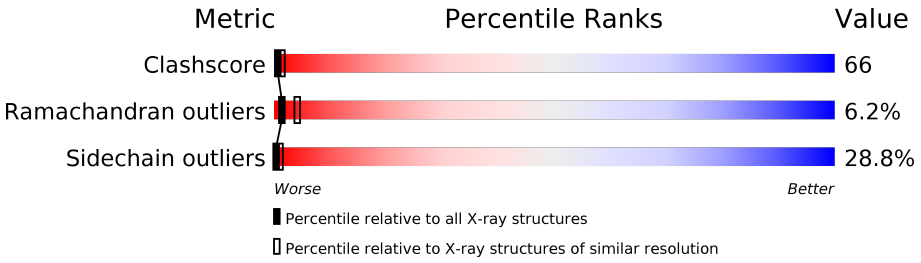
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	584	21% 52% 21% • 6%
1	B	584	20% 49% 25% • 6%
1	C	584	23% 47% 23% • 6%
1	D	584	20% 49% 24% • 6%
1	E	584	22% 53% 19% • 6%
1	F	584	24% 50% 19% • 6%
1	G	584	17% 54% 22% • 6%
1	H	584	23% 50% 20% • 6%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 35527 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called NAD-dependent malic enzyme, mitochondrial.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	551	Total	C	N	O	S	Se	0	0	0
			4344	2781	738	802	9	14			
1	B	551	Total	C	N	O	S	Se	0	0	0
			4344	2781	738	802	9	14			
1	C	551	Total	C	N	O	S	Se	0	0	0
			4344	2781	738	802	9	14			
1	D	551	Total	C	N	O	S	Se	0	0	0
			4344	2781	738	802	9	14			
1	E	551	Total	C	N	O	S	Se	0	0	0
			4344	2781	738	802	9	14			
1	F	551	Total	C	N	O	S	Se	0	0	0
			4344	2781	738	802	9	14			
1	G	551	Total	C	N	O	S	Se	0	0	0
			4344	2781	738	802	9	14			
1	H	551	Total	C	N	O	S	Se	0	0	0
			4344	2781	738	802	9	14			

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	MODIFIED RESIDUE	UNP P23368
A	29	MSE	MET	MODIFIED RESIDUE	UNP P23368
A	38	MSE	MET	MODIFIED RESIDUE	UNP P23368
A	47	MSE	MET	MODIFIED RESIDUE	UNP P23368
A	75	MSE	MET	MODIFIED RESIDUE	UNP P23368
A	86	MSE	MET	MODIFIED RESIDUE	UNP P23368
A	108	MSE	MET	MODIFIED RESIDUE	UNP P23368
A	177	MSE	MET	MODIFIED RESIDUE	UNP P23368
A	219	MSE	MET	MODIFIED RESIDUE	UNP P23368
A	239	MSE	MET	MODIFIED RESIDUE	UNP P23368
A	325	MSE	MET	MODIFIED RESIDUE	UNP P23368
A	327	MSE	MET	MODIFIED RESIDUE	UNP P23368
A	343	MSE	MET	MODIFIED RESIDUE	UNP P23368

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Chain	Residue	Modelled	Actual	Comment	Reference
A	407	MSE	MET	MODIFIED RESIDUE	UNP P23368
A	539	MSE	MET	MODIFIED RESIDUE	UNP P23368
B	1001	MSE	MET	MODIFIED RESIDUE	UNP P23368
B	1029	MSE	MET	MODIFIED RESIDUE	UNP P23368
B	1038	MSE	MET	MODIFIED RESIDUE	UNP P23368
B	1047	MSE	MET	MODIFIED RESIDUE	UNP P23368
B	1075	MSE	MET	MODIFIED RESIDUE	UNP P23368
B	1086	MSE	MET	MODIFIED RESIDUE	UNP P23368
B	1108	MSE	MET	MODIFIED RESIDUE	UNP P23368
B	1177	MSE	MET	MODIFIED RESIDUE	UNP P23368
B	1219	MSE	MET	MODIFIED RESIDUE	UNP P23368
B	1239	MSE	MET	MODIFIED RESIDUE	UNP P23368
B	1325	MSE	MET	MODIFIED RESIDUE	UNP P23368
B	1327	MSE	MET	MODIFIED RESIDUE	UNP P23368
B	1343	MSE	MET	MODIFIED RESIDUE	UNP P23368
B	1407	MSE	MET	MODIFIED RESIDUE	UNP P23368
B	1539	MSE	MET	MODIFIED RESIDUE	UNP P23368
C	2001	MSE	MET	MODIFIED RESIDUE	UNP P23368
C	2029	MSE	MET	MODIFIED RESIDUE	UNP P23368
C	2038	MSE	MET	MODIFIED RESIDUE	UNP P23368
C	2047	MSE	MET	MODIFIED RESIDUE	UNP P23368
C	2075	MSE	MET	MODIFIED RESIDUE	UNP P23368
C	2086	MSE	MET	MODIFIED RESIDUE	UNP P23368
C	2108	MSE	MET	MODIFIED RESIDUE	UNP P23368
C	2177	MSE	MET	MODIFIED RESIDUE	UNP P23368
C	2219	MSE	MET	MODIFIED RESIDUE	UNP P23368
C	2239	MSE	MET	MODIFIED RESIDUE	UNP P23368
C	2325	MSE	MET	MODIFIED RESIDUE	UNP P23368
C	2327	MSE	MET	MODIFIED RESIDUE	UNP P23368
C	2343	MSE	MET	MODIFIED RESIDUE	UNP P23368
C	2407	MSE	MET	MODIFIED RESIDUE	UNP P23368
C	2539	MSE	MET	MODIFIED RESIDUE	UNP P23368
D	3001	MSE	MET	MODIFIED RESIDUE	UNP P23368
D	3029	MSE	MET	MODIFIED RESIDUE	UNP P23368
D	3038	MSE	MET	MODIFIED RESIDUE	UNP P23368
D	3047	MSE	MET	MODIFIED RESIDUE	UNP P23368
D	3075	MSE	MET	MODIFIED RESIDUE	UNP P23368
D	3086	MSE	MET	MODIFIED RESIDUE	UNP P23368
D	3108	MSE	MET	MODIFIED RESIDUE	UNP P23368
D	3177	MSE	MET	MODIFIED RESIDUE	UNP P23368
D	3219	MSE	MET	MODIFIED RESIDUE	UNP P23368
D	3239	MSE	MET	MODIFIED RESIDUE	UNP P23368

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Chain	Residue	Modelled	Actual	Comment	Reference
D	3325	MSE	MET	MODIFIED RESIDUE	UNP P23368
D	3327	MSE	MET	MODIFIED RESIDUE	UNP P23368
D	3343	MSE	MET	MODIFIED RESIDUE	UNP P23368
D	3407	MSE	MET	MODIFIED RESIDUE	UNP P23368
D	3539	MSE	MET	MODIFIED RESIDUE	UNP P23368
E	4001	MSE	MET	MODIFIED RESIDUE	UNP P23368
E	4029	MSE	MET	MODIFIED RESIDUE	UNP P23368
E	4038	MSE	MET	MODIFIED RESIDUE	UNP P23368
E	4047	MSE	MET	MODIFIED RESIDUE	UNP P23368
E	4075	MSE	MET	MODIFIED RESIDUE	UNP P23368
E	4086	MSE	MET	MODIFIED RESIDUE	UNP P23368
E	4108	MSE	MET	MODIFIED RESIDUE	UNP P23368
E	4177	MSE	MET	MODIFIED RESIDUE	UNP P23368
E	4219	MSE	MET	MODIFIED RESIDUE	UNP P23368
E	4239	MSE	MET	MODIFIED RESIDUE	UNP P23368
E	4325	MSE	MET	MODIFIED RESIDUE	UNP P23368
E	4327	MSE	MET	MODIFIED RESIDUE	UNP P23368
E	4343	MSE	MET	MODIFIED RESIDUE	UNP P23368
E	4407	MSE	MET	MODIFIED RESIDUE	UNP P23368
E	4539	MSE	MET	MODIFIED RESIDUE	UNP P23368
F	5001	MSE	MET	MODIFIED RESIDUE	UNP P23368
F	5029	MSE	MET	MODIFIED RESIDUE	UNP P23368
F	5038	MSE	MET	MODIFIED RESIDUE	UNP P23368
F	5047	MSE	MET	MODIFIED RESIDUE	UNP P23368
F	5075	MSE	MET	MODIFIED RESIDUE	UNP P23368
F	5086	MSE	MET	MODIFIED RESIDUE	UNP P23368
F	5108	MSE	MET	MODIFIED RESIDUE	UNP P23368
F	5177	MSE	MET	MODIFIED RESIDUE	UNP P23368
F	5219	MSE	MET	MODIFIED RESIDUE	UNP P23368
F	5239	MSE	MET	MODIFIED RESIDUE	UNP P23368
F	5325	MSE	MET	MODIFIED RESIDUE	UNP P23368
F	5327	MSE	MET	MODIFIED RESIDUE	UNP P23368
F	5343	MSE	MET	MODIFIED RESIDUE	UNP P23368
F	5407	MSE	MET	MODIFIED RESIDUE	UNP P23368
F	5539	MSE	MET	MODIFIED RESIDUE	UNP P23368
G	6001	MSE	MET	MODIFIED RESIDUE	UNP P23368
G	6029	MSE	MET	MODIFIED RESIDUE	UNP P23368
G	6038	MSE	MET	MODIFIED RESIDUE	UNP P23368
G	6047	MSE	MET	MODIFIED RESIDUE	UNP P23368
G	6075	MSE	MET	MODIFIED RESIDUE	UNP P23368
G	6086	MSE	MET	MODIFIED RESIDUE	UNP P23368
G	6108	MSE	MET	MODIFIED RESIDUE	UNP P23368

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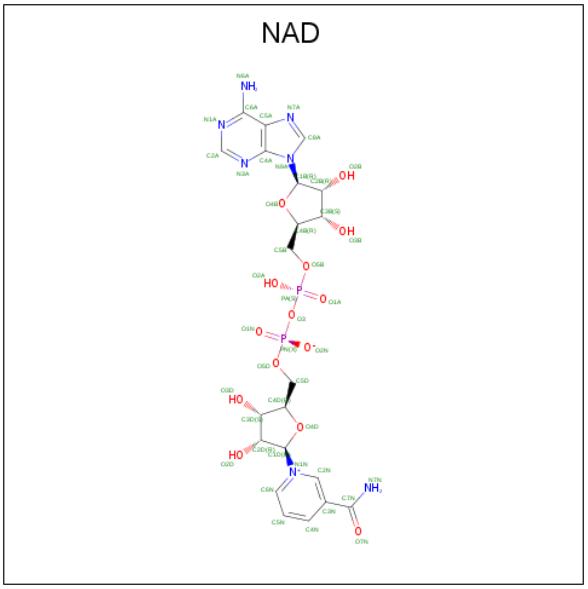
Chain	Residue	Modelled	Actual	Comment	Reference
G	6177	MSE	MET	MODIFIED RESIDUE	UNP P23368
G	6219	MSE	MET	MODIFIED RESIDUE	UNP P23368
G	6239	MSE	MET	MODIFIED RESIDUE	UNP P23368
G	6325	MSE	MET	MODIFIED RESIDUE	UNP P23368
G	6327	MSE	MET	MODIFIED RESIDUE	UNP P23368
G	6343	MSE	MET	MODIFIED RESIDUE	UNP P23368
G	6407	MSE	MET	MODIFIED RESIDUE	UNP P23368
G	6539	MSE	MET	MODIFIED RESIDUE	UNP P23368
H	7001	MSE	MET	MODIFIED RESIDUE	UNP P23368
H	7029	MSE	MET	MODIFIED RESIDUE	UNP P23368
H	7038	MSE	MET	MODIFIED RESIDUE	UNP P23368
H	7047	MSE	MET	MODIFIED RESIDUE	UNP P23368
H	7075	MSE	MET	MODIFIED RESIDUE	UNP P23368
H	7086	MSE	MET	MODIFIED RESIDUE	UNP P23368
H	7108	MSE	MET	MODIFIED RESIDUE	UNP P23368
H	7177	MSE	MET	MODIFIED RESIDUE	UNP P23368
H	7219	MSE	MET	MODIFIED RESIDUE	UNP P23368
H	7239	MSE	MET	MODIFIED RESIDUE	UNP P23368
H	7325	MSE	MET	MODIFIED RESIDUE	UNP P23368
H	7327	MSE	MET	MODIFIED RESIDUE	UNP P23368
H	7343	MSE	MET	MODIFIED RESIDUE	UNP P23368
H	7407	MSE	MET	MODIFIED RESIDUE	UNP P23368
H	7539	MSE	MET	MODIFIED RESIDUE	UNP P23368

- Molecule 2 is LUTETIUM (III) ION (three-letter code: LU) (formula: Lu).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total Lu 1 1	0	0
2	D	1	Total Lu 1 1	0	0
2	E	1	Total Lu 1 1	0	0
2	H	1	Total Lu 1 1	0	0
2	B	1	Total Lu 1 1	0	0
2	C	1	Total Lu 1 1	0	0
2	A	1	Total Lu 1 1	0	0
2	F	1	Total Lu 1 1	0	0

- Molecule 3 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	A	1	Total	C	N	O	P	17	0
			44	21	7	14	2		
3	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	B	1	Total	C	N	O	P	18	0
			44	21	7	14	2		
3	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	C	1	Total	C	N	O	P	18	0
			44	21	7	14	2		
3	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	D	1	Total	C	N	O	P	18	0
			44	21	7	14	2		
3	E	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	E	1	Total	C	N	O	P	18	0
			44	21	7	14	2		
3	F	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	F	1	Total	C	N	O	P	18	0
			44	21	7	14	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	G	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	G	1	Total	C	N	O	P	18	0
			44	21	7	14	2		
3	H	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	H	1	Total	C	N	O	P	18	0
			44	21	7	14	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	9	Total	O	0	0
			9	9		
4	B	6	Total	O	0	0
			6	6		
4	C	11	Total	O	0	0
			11	11		
4	D	6	Total	O	0	0
			6	6		
4	E	6	Total	O	0	0
			6	6		
4	F	10	Total	O	0	0
			10	10		
4	G	5	Total	O	0	0
			5	5		
4	H	10	Total	O	0	0
			10	10		

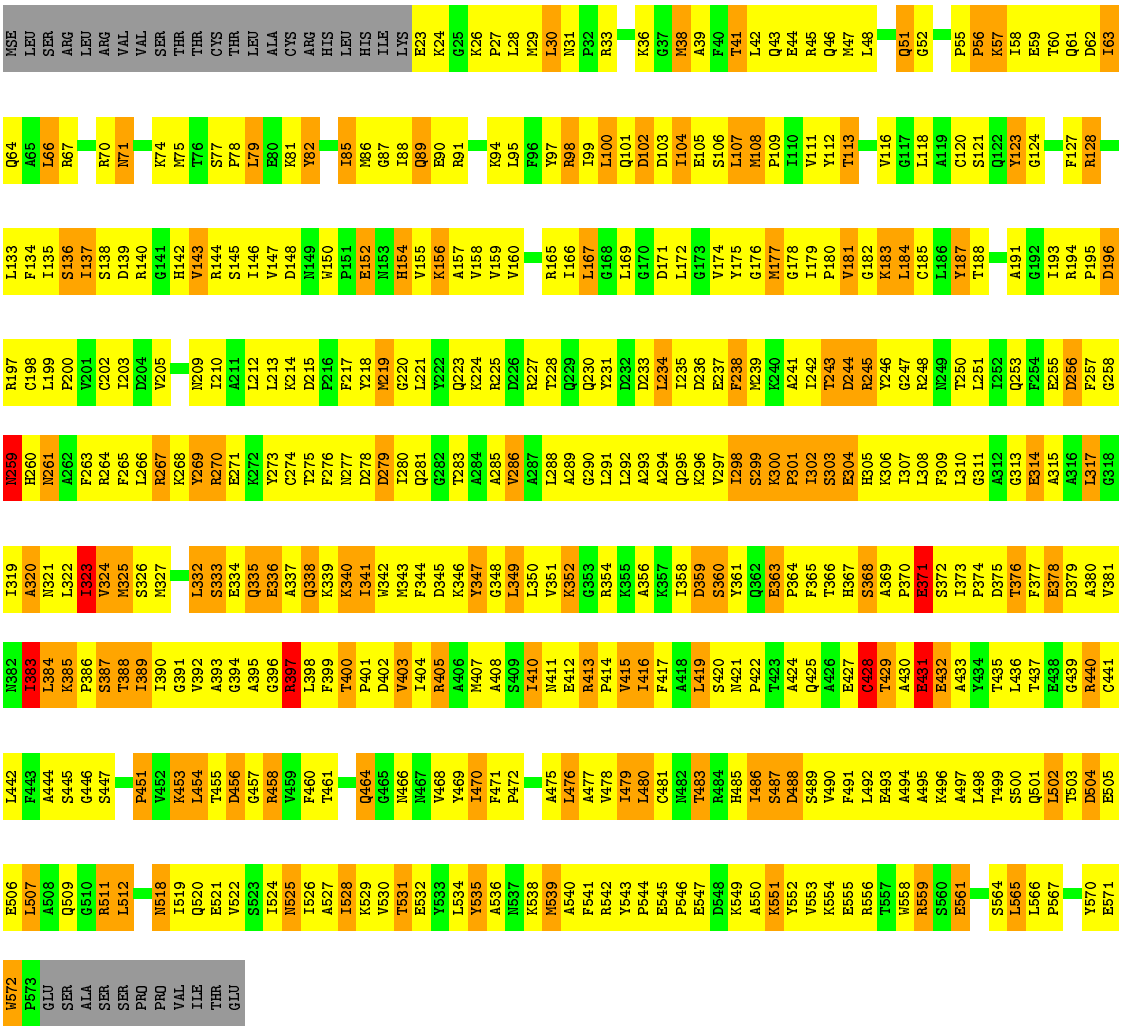
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

Note EDS was not executed.

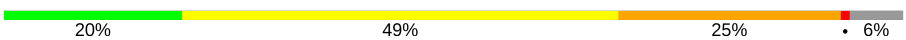
- Molecule 1: NAD-dependent malic enzyme, mitochondrial

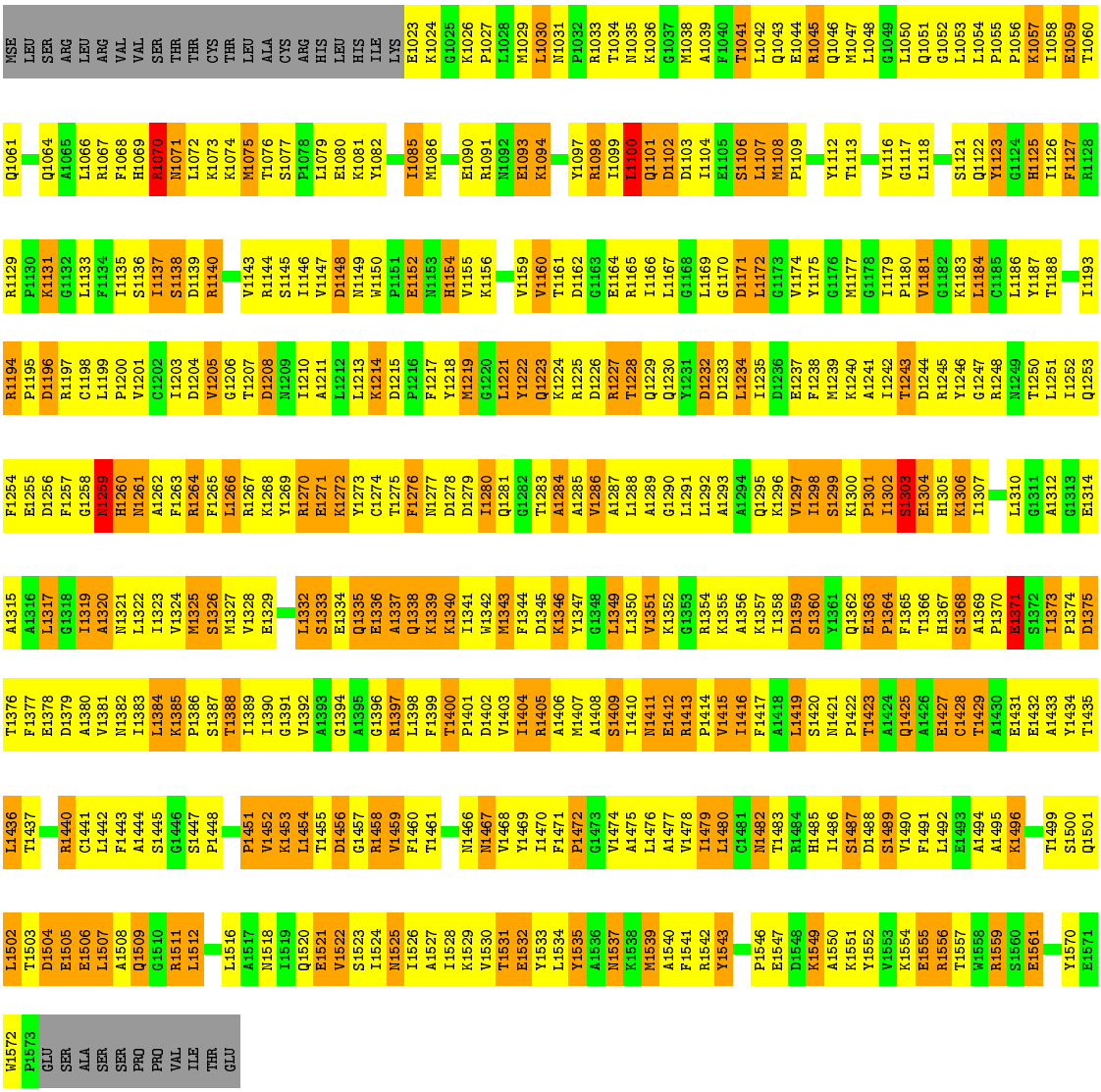
Chain A:



- Molecule 1: NAD-dependent malic enzyme, mitochondrial

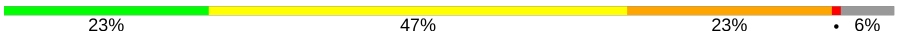
Chain B:

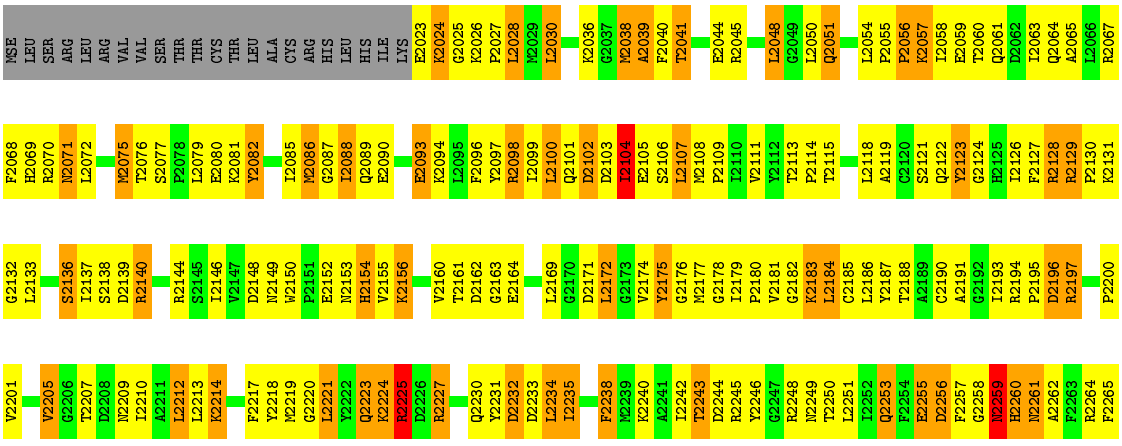


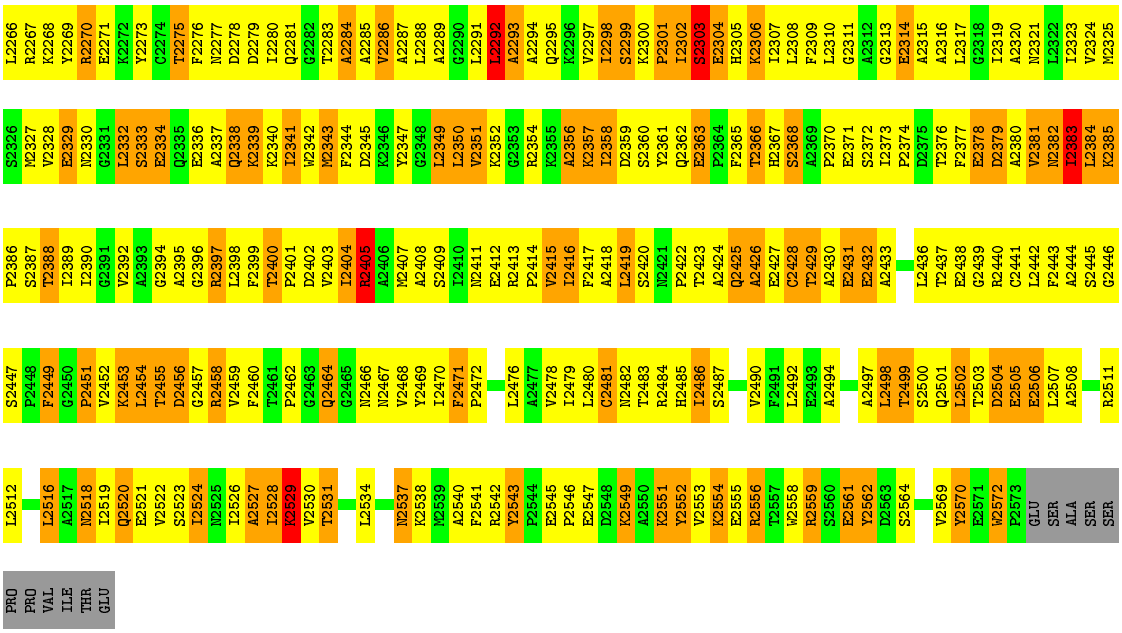


• Molecule 1: NAD-dependent malic enzyme, mitochondrial

Chain C:

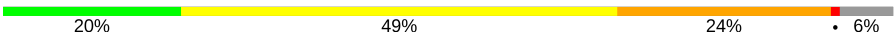


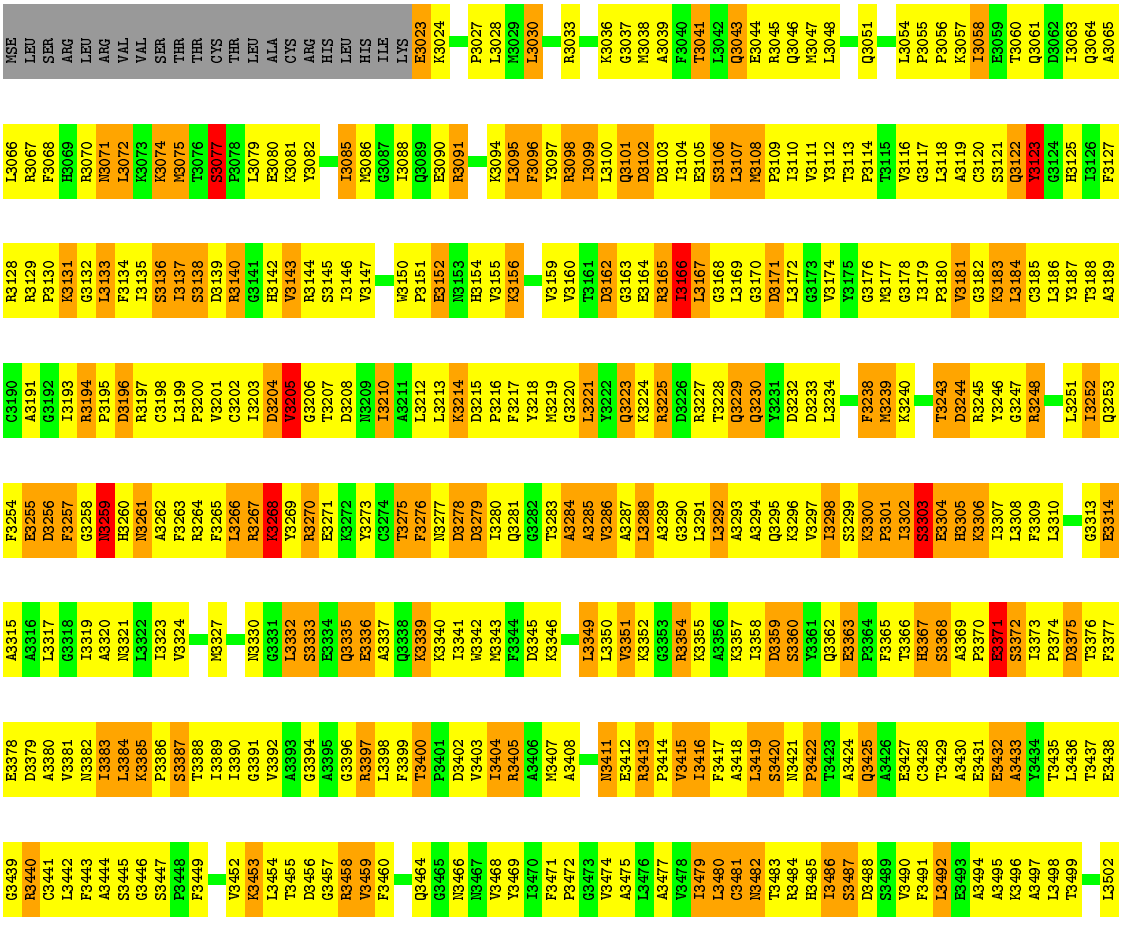




• Molecule 1: NAD-dependent malic enzyme, mitochondrial

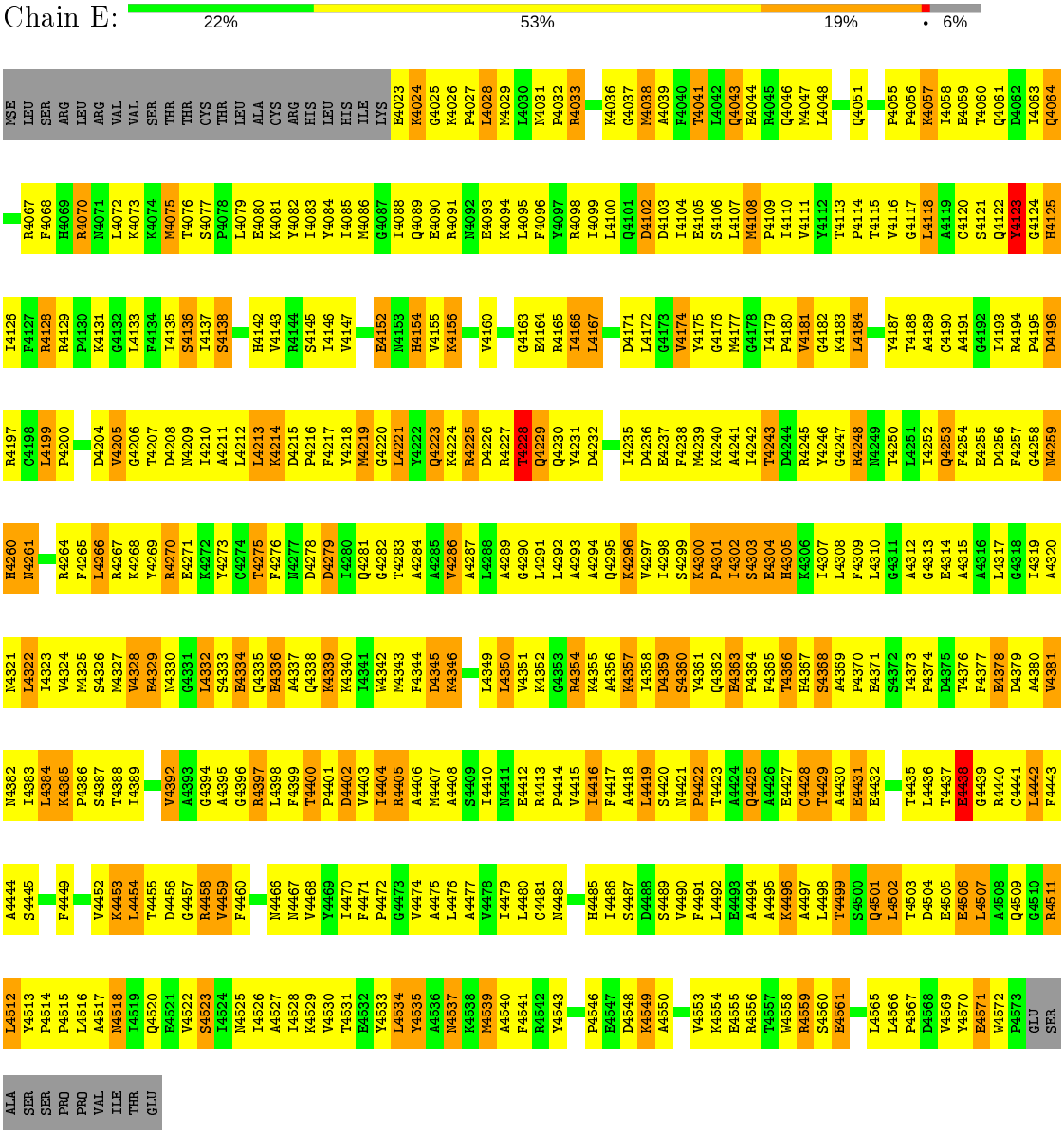
Chain D:





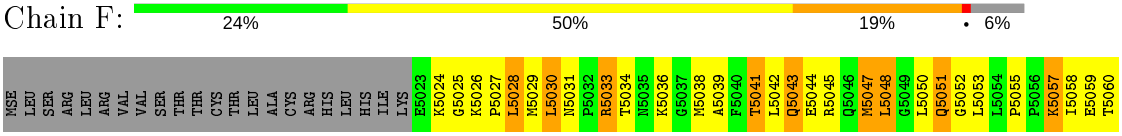
• Molecule 1: NAD-dependent malic enzyme, mitochondrial

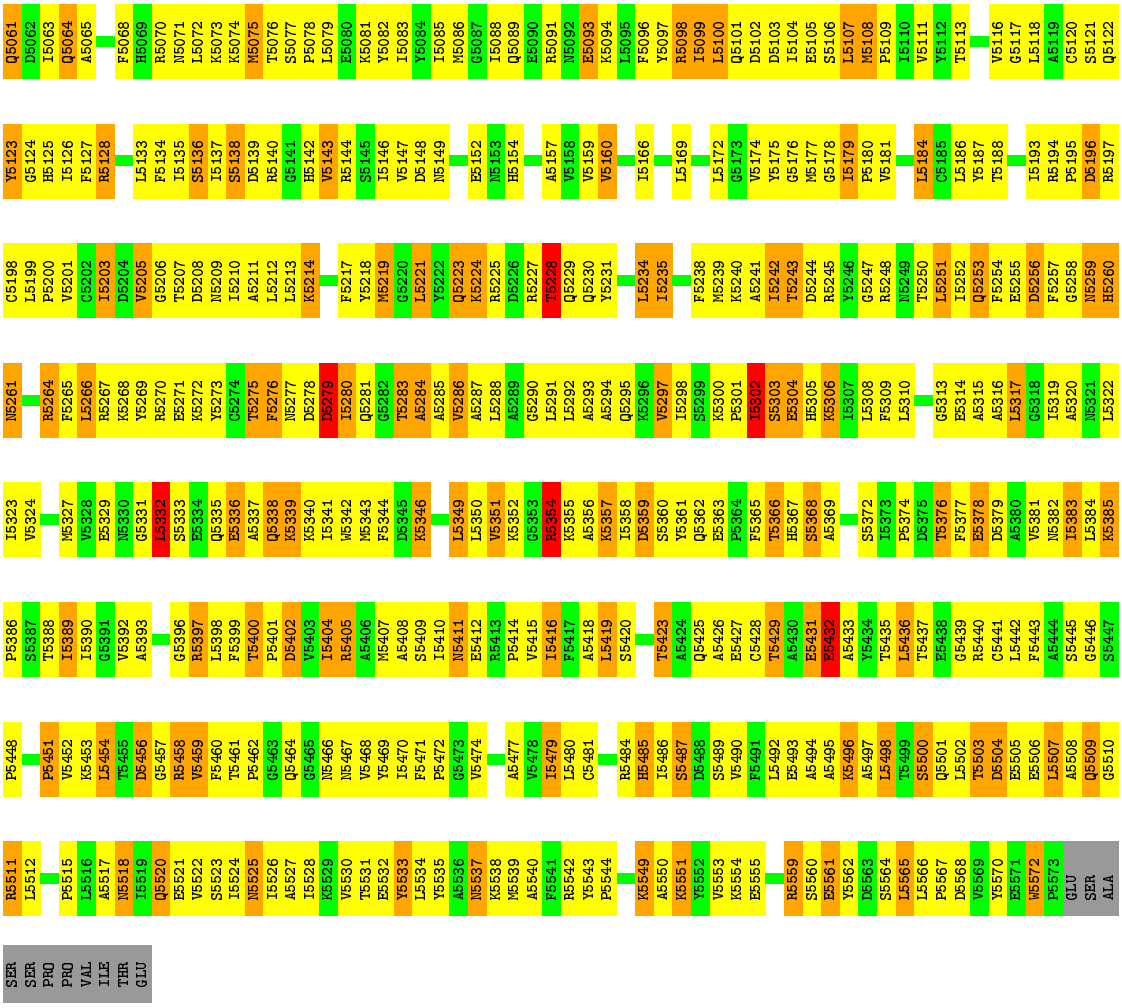
Chain E:



• Molecule 1: NAD-dependent malic enzyme, mitochondrial

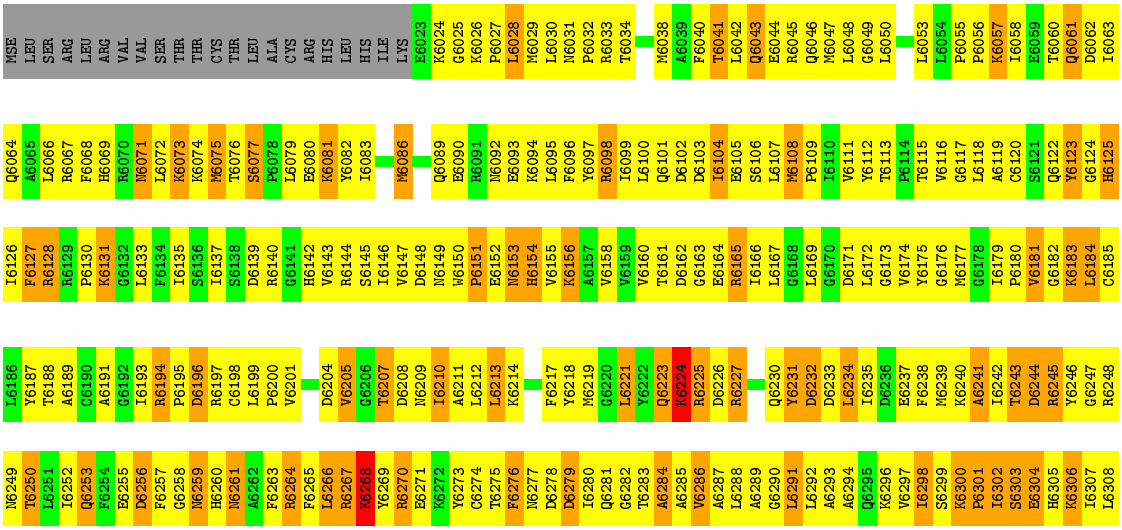
Chain F:

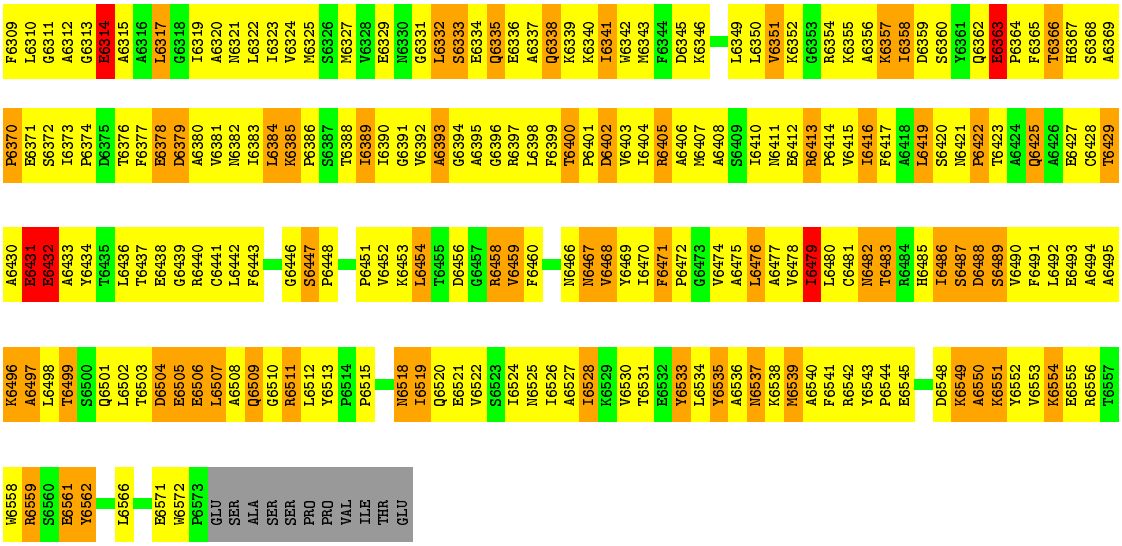




• Molecule 1: NAD-dependent malic enzyme, mitochondrial

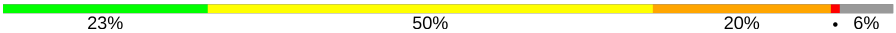
Chain G:

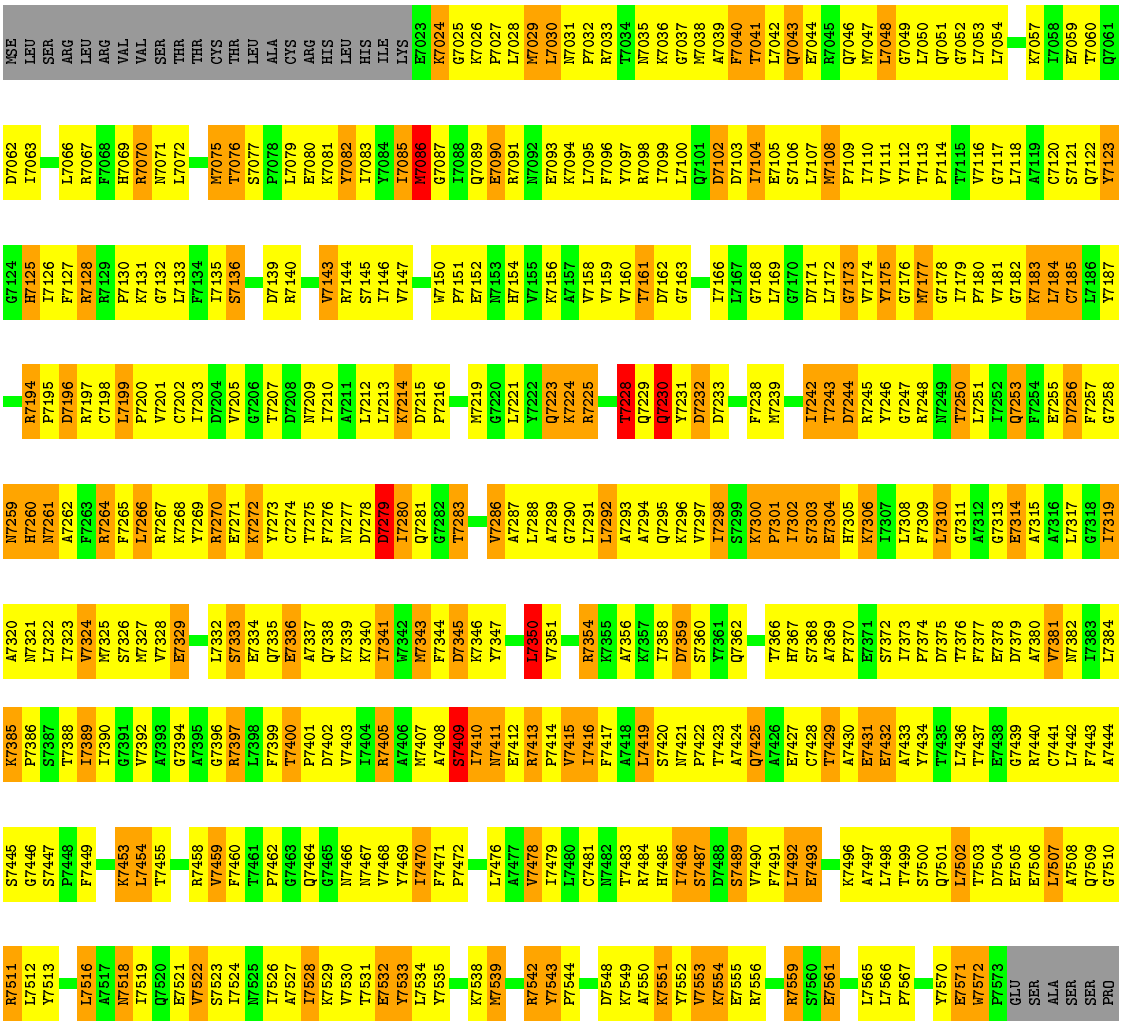




• Molecule 1: NAD-dependent malic enzyme, mitochondrial

Chain H:






PRO
VAL
ILE
THR
GLU

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	113.30Å 119.00Å 125.90Å 116.50° 94.80° 102.80°	Depositor
Resolution (Å)	20.00 – 2.90	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.90)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.204 , 0.263	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	35527	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.46	0/4424	0.67	0/5969
1	B	0.46	0/4424	0.66	0/5969
1	C	0.46	0/4424	0.66	0/5969
1	D	0.49	0/4424	0.69	0/5969
1	E	0.47	0/4424	0.68	1/5969 (0.0%)
1	F	0.47	0/4424	0.66	0/5969
1	G	0.46	0/4424	0.69	0/5969
1	H	0.46	0/4424	0.68	0/5969
All	All	0.47	0/35392	0.67	1/47752 (0.0%)

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

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

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	4442	LEU	CA-CB-CG	-5.11	103.55	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	187	TYR	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4344	0	4372	604	0
1	B	4344	0	4372	618	0
1	C	4344	0	4372	594	0
1	D	4344	0	4372	650	0
1	E	4344	0	4372	543	0
1	F	4344	0	4372	504	0
1	G	4344	0	4372	654	0
1	H	4344	0	4372	560	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	88	0	52	3	0
3	B	88	0	52	5	0
3	C	88	0	52	2	0
3	D	88	0	52	4	0
3	E	88	0	52	3	0
3	F	88	0	52	3	0
3	G	88	0	52	4	0
3	H	88	0	52	3	0
4	A	9	0	0	3	0
4	B	6	0	0	1	0
4	C	11	0	0	1	0
4	D	6	0	0	6	0
4	E	6	0	0	0	0
4	F	10	0	0	1	0
4	G	5	0	0	3	0
4	H	10	0	0	1	0
All	All	35527	0	35392	4647	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 66.

All (4647) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3061:GLN:HA	1:D:3064:GLN:HE21	1.04	1.18
1:D:3388:THR:HG23	1:D:3415:VAL:HB	1.27	1.15
1:H:7388:THR:HG23	1:H:7415:VAL:HB	1.27	1.14
1:D:3253:GLN:HE22	1:D:3255:GLU:HG2	1.13	1.13
1:D:3263:PHE:HA	4:D:8022:HOH:O	1.48	1.13
1:H:7210:ILE:HG22	1:H:7214:LYS:HZ1	1.01	1.13
1:A:61:GLN:HA	1:A:64:GLN:HE21	1.15	1.10
1:H:7210:ILE:HG22	1:H:7214:LYS:NZ	1.66	1.10
1:D:3041:THR:HG23	1:D:3044:GLU:HG3	1.33	1.09
1:D:3177:MSE:HE1	1:D:3200:PRO:HB2	1.34	1.09
1:A:243:THR:HB	1:A:248:ARG:HD2	1.17	1.09
1:C:2197:ARG:HG2	1:C:2197:ARG:HH11	1.09	1.08
1:D:3437:THR:HG21	1:D:3441:CYS:HB3	1.35	1.08
1:G:6240:LYS:HG3	1:G:6248:ARG:HH22	1.19	1.07
1:H:7415:VAL:HG13	1:H:7442:LEU:HB2	1.36	1.07
1:D:3144:ARG:NH1	1:D:3244:ASP:HB3	1.69	1.06
1:G:6205:VAL:HG12	1:G:6226:ASP:HB3	1.39	1.05
1:E:4177:MSE:HE1	1:E:4200:PRO:HB2	1.38	1.04
1:F:5177:MSE:HE1	1:F:5200:PRO:HB2	1.40	1.03
1:C:2227:ARG:HG2	1:C:2227:ARG:HH11	1.22	1.03
1:G:6317:LEU:H	1:G:6317:LEU:HD12	1.23	1.03
1:B:1177:MSE:O	1:B:1180:PRO:HD2	1.58	1.03
1:G:6160:VAL:HG12	1:G:6201:VAL:HB	1.42	1.01
1:H:7325:MSE:HE1	1:H:7489:SER:HA	1.41	1.01
1:G:6323:ILE:HG22	1:G:6327:MSE:HE2	1.40	1.01
1:H:7466:ASN:HB3	1:H:7468:VAL:HG12	1.40	1.01
1:C:2128:ARG:HH11	1:C:2128:ARG:HG2	1.23	1.01
1:B:1166:ILE:HD12	1:B:1179:ILE:HG13	1.41	1.01
1:D:3369:ALA:HB1	1:D:3373:ILE:HD11	1.43	1.01
1:B:1388:THR:HG23	1:B:1415:VAL:HB	1.43	1.00
1:F:5388:THR:HG23	1:F:5415:VAL:HB	1.42	1.00
1:H:7408:ALA:HB2	1:H:7437:THR:HG22	1.43	1.00
1:C:2104:ILE:HG13	1:C:2108:MSE:HE2	1.43	1.00
1:F:5453:LYS:HB2	1:F:5459:VAL:HG13	1.39	1.00
1:G:6177:MSE:HE1	1:G:6200:PRO:HB2	1.40	1.00
1:D:3421:ASN:HA	1:D:3422:PRO:O	1.61	1.00
1:G:6243:THR:HB	1:G:6248:ARG:HD2	1.43	0.99
1:H:7177:MSE:HE1	1:H:7200:PRO:HB2	1.44	0.99
1:B:1338:GLN:HG3	1:B:1364:PRO:O	1.62	0.98
1:F:5572:TRP:HB2	1:H:7042:LEU:HD21	1.46	0.98
1:E:4240:LYS:HG3	1:E:4248:ARG:HH22	1.27	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1317:LEU:HD12	1:B:1317:LEU:H	1.28	0.98
1:B:1210:ILE:HA	1:B:1213:LEU:HD12	1.46	0.98
1:D:3065:ALA:HA	1:D:3099:ILE:HD11	1.44	0.97
1:F:5269:TYR:HB3	1:F:5273:TYR:HD1	1.27	0.97
1:G:6327:MSE:HE1	1:G:6341:ILE:HD11	1.41	0.97
1:A:454:LEU:HD13	1:A:458:ARG:NH1	1.79	0.97
1:D:3374:PRO:HD3	1:D:3383:ILE:HD12	1.47	0.96
1:C:2306:LYS:HB3	1:C:2386:PRO:HA	1.46	0.96
1:H:7377:PHE:HZ	1:H:7389:ILE:HD11	1.30	0.96
1:B:1429:THR:HG23	1:B:1432:GLU:HG3	1.48	0.96
1:F:5128:ARG:HH11	1:F:5128:ARG:HG2	1.31	0.96
1:B:1298:ILE:HD11	1:B:1442:LEU:HD11	1.48	0.95
1:F:5109:PRO:HA	1:F:5113:THR:O	1.66	0.95
1:F:5317:LEU:H	1:F:5317:LEU:HD12	1.30	0.95
1:G:6103:ASP:HB3	1:G:6107:LEU:HD23	1.47	0.95
1:B:1227:ARG:HG2	1:B:1227:ARG:HH11	1.32	0.95
1:E:4174:VAL:HG23	1:E:4219:MSE:HE3	1.48	0.95
1:A:298:ILE:HD11	1:A:442:LEU:HD11	1.49	0.95
1:G:6454:LEU:HD12	1:G:6458:ARG:HB3	1.45	0.95
1:G:6144:ARG:NH1	1:G:6244:ASP:HB3	1.82	0.95
1:D:3218:TYR:HE2	4:D:8046:HOH:O	1.49	0.94
1:D:3027:PRO:HA	1:D:3030:LEU:HB2	1.47	0.94
1:C:2317:LEU:H	1:C:2317:LEU:HD12	1.30	0.94
1:E:4360:SER:HA	1:E:4363:GLU:OE1	1.67	0.94
1:A:419:LEU:H	1:A:419:LEU:HD22	1.31	0.94
1:D:3283:THR:O	1:D:3286:VAL:HG23	1.67	0.94
1:B:1306:LYS:HB3	1:B:1386:PRO:HA	1.50	0.94
1:D:3210:ILE:HA	1:D:3213:LEU:HD12	1.49	0.93
1:B:1466:ASN:HB3	1:B:1468:VAL:HG12	1.50	0.93
1:G:6421:ASN:HA	1:G:6422:PRO:O	1.67	0.93
1:E:4453:LYS:HG2	1:E:4459:VAL:HG13	1.50	0.93
1:A:327:MSE:HE3	1:A:337:ALA:HB1	1.49	0.93
1:A:317:LEU:H	1:A:317:LEU:HD12	1.30	0.93
1:B:1402:ASP:HA	1:B:1405:ARG:HD2	1.50	0.92
1:G:6360:SER:HA	1:G:6363:GLU:HG2	1.50	0.92
1:E:4421:ASN:HA	1:E:4422:PRO:O	1.69	0.92
1:B:1399:PHE:HA	1:B:1403:VAL:HG11	1.50	0.92
1:F:5453:LYS:HE3	1:F:5457:GLY:HA2	1.52	0.92
1:A:466:ASN:HB3	1:A:468:VAL:HG12	1.52	0.92
1:D:3075:MSE:HB3	1:D:3081:LYS:HD3	1.50	0.92
1:E:4407:MSE:HA	1:E:4410:ILE:HD12	1.51	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:4454:LEU:HD12	1:E:4458:ARG:O	1.69	0.92
1:G:6038:MSE:HE3	1:G:6055:PRO:HG2	1.52	0.91
1:A:128:ARG:HH11	1:A:128:ARG:HG2	1.36	0.91
1:D:3156:LYS:HB3	1:D:3479:ILE:HD12	1.48	0.91
1:G:6388:THR:HG23	1:G:6415:VAL:HB	1.52	0.91
1:G:6489:SER:HG	1:G:6533:TYR:HH	1.17	0.91
1:G:6079:LEU:HD13	1:G:6118:LEU:HD22	1.53	0.91
1:H:7177:MSE:CE	1:H:7200:PRO:HB2	2.00	0.91
1:F:5559:ARG:HB3	1:F:5561:GLU:HG2	1.52	0.91
1:B:1240:LYS:HG3	1:B:1248:ARG:HH22	1.34	0.91
1:G:6416:ILE:H	1:G:6416:ILE:HD13	1.33	0.91
1:E:4061:GLN:HA	1:E:4064:GLN:HE21	1.35	0.90
1:F:5179:ILE:HB	1:F:5180:PRO:HD3	1.52	0.90
1:F:5137:ILE:HA	1:F:5234:LEU:CD2	2.01	0.90
1:D:3243:THR:HB	1:D:3248:ARG:HD2	1.51	0.90
1:G:6559:ARG:HB3	1:G:6561:GLU:HG2	1.53	0.90
1:E:4026:LYS:HA	1:E:4029:MSE:HE2	1.53	0.90
1:A:402:ASP:HA	1:A:405:ARG:HD2	1.54	0.90
1:A:527:ALA:O	1:A:531:THR:HG23	1.72	0.90
1:C:2210:ILE:HA	1:C:2213:LEU:HD12	1.54	0.90
1:C:2056:PRO:HG2	1:D:3220:GLY:HA2	1.53	0.90
1:G:6354:ARG:HE	1:G:6356:ALA:HB3	1.37	0.90
1:G:6404:ILE:HB	1:G:6436:LEU:HD23	1.54	0.90
1:C:2261:ASN:H	1:C:2261:ASN:HD22	1.15	0.89
1:H:7327:MSE:HE3	1:H:7337:ALA:HB1	1.55	0.89
1:D:3061:GLN:HA	1:D:3064:GLN:NE2	1.87	0.89
1:G:6253:GLN:NE2	1:G:6278:ASP:HB2	1.87	0.89
1:H:7243:THR:HB	1:H:7248:ARG:HD2	1.55	0.89
1:H:7369:ALA:HB1	1:H:7373:ILE:HD11	1.55	0.89
1:A:451:PRO:HA	1:A:460:PHE:O	1.71	0.89
1:E:4350:LEU:HD22	1:E:4354:ARG:NH1	1.87	0.89
1:F:5309:PHE:HB2	1:F:5343:MSE:HG2	1.55	0.89
1:A:401:PRO:HA	1:A:404:ILE:HD12	1.54	0.89
1:B:1261:ASN:H	1:B:1261:ASN:ND2	1.60	0.88
1:C:2453:LYS:HA	1:C:2458:ARG:O	1.73	0.88
1:D:3402:ASP:HA	1:D:3405:ARG:HD2	1.55	0.88
1:F:5137:ILE:HA	1:F:5234:LEU:HD21	1.55	0.88
1:C:2439:GLY:HA3	1:C:2460:PHE:HE2	1.34	0.88
1:G:6043:GLN:HG2	1:G:6566:LEU:HD11	1.56	0.88
1:C:2332:LEU:HD23	1:C:2336:GLU:HG3	1.53	0.88
1:B:1204:ASP:OD1	1:B:1221:LEU:HB2	1.73	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:PHE:HB2	1:A:427:GLU:O	1.74	0.88
1:D:3319:ILE:HG22	1:D:3323:ILE:HD11	1.54	0.88
1:A:243:THR:HB	1:A:248:ARG:CD	2.02	0.87
1:B:1253:GLN:HG3	1:B:1276:PHE:CZ	2.08	0.87
1:E:4113:THR:HA	1:E:4116:VAL:HG12	1.55	0.87
1:F:5251:LEU:HD12	1:F:5252:ILE:N	1.88	0.87
1:A:559:ARG:HG3	1:A:561:GLU:HG2	1.56	0.87
1:E:4261:ASN:H	1:E:4261:ASN:ND2	1.72	0.87
1:F:5360:SER:HA	1:F:5363:GLU:OE1	1.72	0.87
1:A:61:GLN:HA	1:A:64:GLN:NE2	1.90	0.87
1:C:2197:ARG:HG2	1:C:2197:ARG:NH1	1.85	0.86
1:C:2315:ALA:HB3	1:C:2392:VAL:HG11	1.57	0.86
1:C:2051:GLN:HA	1:C:2051:GLN:HE21	1.40	0.86
1:B:1394:GLY:O	1:B:1425:GLN:HG3	1.74	0.86
1:G:6177:MSE:CE	1:G:6200:PRO:HB2	2.05	0.86
1:G:6123:TYR:HD2	1:G:6219:MSE:HE1	1.37	0.86
1:H:7179:ILE:HB	1:H:7180:PRO:HD3	1.55	0.86
1:E:4072:LEU:HA	1:E:4075:MSE:HE3	1.57	0.86
1:C:2307:ILE:HG13	1:C:2388:THR:HB	1.57	0.86
1:G:6493:GLU:HA	1:G:6496:LYS:HD3	1.57	0.86
1:D:3097:TYR:O	1:D:3101:GLN:HG3	1.76	0.86
1:E:4531:THR:HA	1:E:4534:LEU:HD12	1.56	0.85
1:H:7043:GLN:HG2	1:H:7566:LEU:HD11	1.57	0.85
1:E:4164:GLU:HG3	1:E:4225:ARG:CZ	2.06	0.85
1:E:4298:ILE:HD11	1:E:4442:LEU:HD11	1.55	0.85
1:G:6354:ARG:NE	1:G:6356:ALA:HB3	1.91	0.85
1:G:6478:VAL:HG12	1:G:6479:ILE:HD13	1.57	0.85
1:A:428:CYS:SG	1:A:429:THR:N	2.50	0.85
1:G:6086:MSE:HE2	1:G:6086:MSE:HA	1.58	0.85
1:H:7109:PRO:HA	1:H:7113:THR:O	1.76	0.85
1:C:2219:MSE:HG2	1:D:3038:MSE:HE1	1.58	0.85
1:B:1401:PRO:HA	1:B:1404:ILE:HD12	1.59	0.85
1:C:2382:ASN:O	1:C:2385:LYS:HG3	1.77	0.85
1:A:51:GLN:HE21	1:A:51:GLN:HA	1.40	0.85
1:H:7182:GLY:O	1:H:7185:CYS:HB2	1.76	0.85
1:H:7210:ILE:CG2	1:H:7214:LYS:HZ1	1.89	0.85
1:C:2438:GLU:HB2	1:C:2440:ARG:HG3	1.59	0.85
1:E:4261:ASN:HD22	1:E:4261:ASN:H	1.23	0.85
1:F:5354:ARG:HE	1:F:5356:ALA:HB3	1.42	0.85
1:G:6086:MSE:CE	1:G:6086:MSE:HA	2.07	0.85
1:D:3144:ARG:HH12	1:D:3244:ASP:HB3	1.41	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2128:ARG:HH11	1:C:2128:ARG:CG	1.89	0.84
1:F:5456:ASP:HB2	1:F:5458:ARG:HD3	1.59	0.84
1:A:103:ASP:HB3	1:A:107:LEU:HD22	1.58	0.84
1:B:1351:VAL:HG21	1:B:1369:ALA:HA	1.58	0.84
1:A:454:LEU:H	1:A:454:LEU:HD12	1.39	0.84
1:D:3041:THR:HG23	1:D:3044:GLU:CG	2.06	0.84
1:A:408:ALA:HA	1:A:414:PRO:HG3	1.59	0.84
1:E:4116:VAL:HG21	1:E:4179:ILE:HD13	1.60	0.84
1:H:7266:LEU:O	1:H:7270:ARG:HB3	1.78	0.84
1:A:109:PRO:HA	1:A:113:THR:O	1.77	0.84
1:D:3043:GLN:HG2	1:D:3566:LEU:HD11	1.59	0.84
1:F:5303:SER:HA	1:F:5340:LYS:HZ2	1.42	0.84
1:E:4400:THR:HG23	1:E:4403:VAL:HG23	1.57	0.83
1:B:1503:THR:HG23	1:B:1506:GLU:OE1	1.76	0.83
1:C:2351:VAL:HG21	1:C:2370:PRO:HD3	1.60	0.83
1:D:3253:GLN:NE2	1:D:3255:GLU:HG2	1.92	0.83
1:D:3466:ASN:HB3	1:D:3468:VAL:HG12	1.59	0.83
1:D:3471:PHE:CD2	1:D:3472:PRO:HD3	2.13	0.83
1:B:1335:GLN:NE2	1:B:1339:LYS:HG3	1.94	0.83
1:H:7394:GLY:HA2	1:H:7420:SER:HB3	1.61	0.83
1:B:1253:GLN:NE2	1:B:1255:GLU:HG2	1.94	0.83
1:C:2207:THR:O	1:C:2224:LYS:HA	1.79	0.83
1:F:5322:LEU:HD11	1:F:5492:LEU:HB2	1.61	0.83
1:C:2416:ILE:HD13	1:C:2416:ILE:H	1.43	0.83
1:H:7388:THR:CG2	1:H:7415:VAL:HB	2.08	0.83
1:A:276:PHE:HB2	1:A:281:GLN:NE2	1.94	0.82
1:A:343:MSE:O	1:A:350:LEU:HB2	1.79	0.82
1:B:1160:VAL:HG13	1:B:1201:VAL:HB	1.60	0.82
1:B:1503:THR:OG1	1:B:1506:GLU:HB2	1.78	0.82
1:C:2419:LEU:N	1:C:2419:LEU:HD22	1.94	0.82
1:D:3320:ALA:HA	1:D:3323:ILE:HD12	1.61	0.82
1:F:5487:SER:O	1:F:5490:VAL:HG23	1.78	0.82
1:G:6352:LYS:HG3	1:G:6368:SER:HA	1.60	0.82
1:G:6454:LEU:HD11	1:G:6460:PHE:CE2	2.14	0.82
1:B:1307:ILE:HG12	1:B:1388:THR:HB	1.62	0.82
1:E:4428:CYS:SG	1:E:4429:THR:N	2.51	0.82
1:F:5253:GLN:HG3	1:F:5276:PHE:CZ	2.14	0.82
1:G:6240:LYS:CG	1:G:6248:ARG:HH22	1.91	0.82
1:A:59:GLU:HG2	1:A:63:ILE:HG21	1.61	0.82
1:D:3177:MSE:O	1:D:3180:PRO:HD2	1.78	0.82
1:A:518:ASN:O	1:A:522:VAL:HG23	1.80	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:4122:GLN:O	1:E:4125:HIS:HB2	1.78	0.82
1:B:1389:ILE:HG22	1:B:1416:ILE:HA	1.59	0.82
1:D:3342:TRP:HZ3	1:D:3351:VAL:HG23	1.42	0.82
1:E:4359:ASP:OD2	1:E:4362:GLN:HG3	1.80	0.82
1:H:7060:THR:HG23	1:H:7063:ILE:HD11	1.59	0.82
1:C:2388:THR:HG23	1:C:2415:VAL:HB	1.61	0.82
1:D:3257:PHE:HB3	1:D:3262:ALA:HB2	1.60	0.82
1:H:7086:MSE:HA	1:H:7086:MSE:HE2	1.62	0.81
1:F:5528:ILE:HD13	1:F:5550:ALA:HA	1.63	0.81
1:G:6267:ARG:HH11	1:G:6267:ARG:HG3	1.46	0.81
1:C:2413:ARG:HA	1:C:2440:ARG:O	1.81	0.81
1:D:3468:VAL:HA	1:D:3471:PHE:CE2	2.15	0.81
1:D:3526:ILE:O	1:D:3530:VAL:HG23	1.80	0.81
1:F:5416:ILE:HD13	1:F:5442:LEU:O	1.79	0.81
1:D:3518:ASN:HB3	1:D:3521:GLU:OE2	1.80	0.81
1:E:4466:ASN:HB3	1:E:4468:VAL:HG12	1.62	0.81
1:A:402:ASP:O	1:A:405:ARG:HG2	1.80	0.81
1:A:419:LEU:N	1:A:419:LEU:HD22	1.96	0.81
1:D:3177:MSE:HE2	1:D:3181:VAL:HG22	1.63	0.81
1:D:3389:ILE:HG22	1:D:3416:ILE:HG22	1.61	0.81
1:F:5194:ARG:HB2	1:F:5197:ARG:HG2	1.62	0.81
1:H:7415:VAL:HG22	1:H:7442:LEU:HD12	1.62	0.81
1:D:3300:LYS:HZ1	1:D:3305:HIS:HA	1.46	0.81
1:G:6126:ILE:HG13	4:G:8062:HOH:O	1.80	0.81
1:C:2109:PRO:HA	1:C:2113:THR:O	1.81	0.80
1:C:2432:GLU:HA	1:C:2436:LEU:HD13	1.61	0.80
1:E:4166:ILE:HG21	1:E:4172:LEU:HD12	1.60	0.80
1:E:4308:LEU:HB3	1:E:4389:ILE:CD1	2.11	0.80
1:A:392:VAL:HG23	1:A:419:LEU:HD23	1.62	0.80
1:D:3072:LEU:HD11	1:D:3081:LYS:HB3	1.63	0.80
1:G:6408:ALA:HB2	1:G:6437:THR:HG22	1.63	0.80
1:H:7478:VAL:HG13	1:H:7483:THR:HB	1.63	0.80
1:F:5057:LYS:C	1:F:5058:ILE:HD13	2.00	0.80
1:B:1061:GLN:HA	1:B:1064:GLN:HE21	1.47	0.80
1:C:2487:SER:O	1:C:2490:VAL:HG23	1.82	0.80
1:C:2569:VAL:HG12	1:C:2570:TYR:N	1.97	0.80
1:G:6490:VAL:HG22	1:G:6533:TYR:HE2	1.47	0.80
1:D:3378:GLU:HG3	1:D:3379:ASP:N	1.95	0.80
1:G:6024:LYS:HA	1:G:6028:LEU:HD22	1.61	0.80
1:A:378:GLU:HB2	1:A:403:VAL:HG23	1.63	0.80
1:B:1392:VAL:HG23	1:B:1419:LEU:HD23	1.64	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1502:LEU:HD12	1:B:1506:GLU:HB3	1.64	0.80
1:C:2060:THR:O	1:C:2064:GLN:HG3	1.82	0.80
1:C:2038:MSE:CB	1:C:2059:GLU:HG3	2.12	0.80
1:C:2419:LEU:H	1:C:2419:LEU:HD22	1.47	0.80
1:B:1271:GLU:OE2	1:B:1271:GLU:HA	1.82	0.80
1:D:3471:PHE:CG	1:D:3472:PRO:HD3	2.17	0.80
1:G:6369:ALA:HB1	1:G:6373:ILE:HD11	1.62	0.79
1:B:1452:VAL:O	1:B:1459:VAL:HA	1.82	0.79
1:C:2123:TYR:HD2	1:C:2219:MSE:HE1	1.47	0.79
1:G:6320:ALA:HB1	1:G:6365:PHE:CE2	2.17	0.79
1:C:2343:MSE:O	1:C:2350:LEU:HB2	1.82	0.79
1:E:4374:PRO:HG3	1:E:4380:ALA:HA	1.65	0.79
1:F:5354:ARG:HG2	1:F:5358:ILE:HD11	1.64	0.79
1:H:7526:ILE:O	1:H:7530:VAL:HG23	1.82	0.79
1:F:5166:ILE:HD12	1:F:5179:ILE:HG13	1.65	0.79
1:F:5315:ALA:O	1:F:5319:ILE:HD12	1.82	0.79
1:H:7412:GLU:HA	1:H:7440:ARG:NH1	1.98	0.79
1:A:512:LEU:HD12	1:A:512:LEU:N	1.98	0.79
1:A:128:ARG:HG3	1:B:1091:ARG:NH1	1.98	0.79
1:C:2569:VAL:HG12	1:C:2570:TYR:H	1.45	0.79
1:D:3239:MSE:HE3	1:D:3273:TYR:HD1	1.48	0.79
1:D:3531:THR:HA	1:D:3534:LEU:HD12	1.63	0.79
1:G:6253:GLN:HG3	1:G:6276:PHE:CZ	2.18	0.79
1:C:2466:ASN:HB3	1:C:2468:VAL:HG12	1.65	0.79
1:F:5128:ARG:NH1	1:F:5128:ARG:HG2	1.94	0.79
1:C:2227:ARG:CG	1:C:2227:ARG:HH11	1.95	0.79
1:F:5515:PRO:HG2	1:F:5518:ASN:OD1	1.83	0.79
1:F:5401:PRO:HA	1:F:5404:ILE:HD12	1.64	0.78
1:A:243:THR:HG22	1:A:248:ARG:HA	1.64	0.78
1:C:2041:THR:HG23	1:C:2044:GLU:OE2	1.84	0.78
1:D:3477:ALA:HB1	1:D:3531:THR:HG22	1.64	0.78
1:C:2298:ILE:HD11	1:C:2442:LEU:HD11	1.65	0.78
1:D:3372:SER:HB2	1:D:3383:ILE:HD13	1.64	0.78
1:D:3468:VAL:HA	1:D:3471:PHE:HE2	1.48	0.78
1:F:5120:CYS:O	1:F:5123:TYR:HB2	1.84	0.78
1:G:6401:PRO:HA	1:G:6436:LEU:HD21	1.65	0.78
1:H:7310:LEU:O	1:H:7310:LEU:HD12	1.83	0.78
1:H:7327:MSE:HE1	1:H:7337:ALA:O	1.83	0.78
1:A:288:LEU:HA	1:A:291:LEU:HB2	1.63	0.78
1:C:2210:ILE:HG22	1:C:2214:LYS:HD2	1.66	0.78
1:B:1421:ASN:HA	1:B:1422:PRO:O	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3298:ILE:HD11	1:D:3442:LEU:HD11	1.66	0.78
1:F:5323:ILE:HG22	1:F:5327:MSE:HE2	1.64	0.78
1:B:1177:MSE:HE1	1:B:1200:PRO:HB2	1.66	0.78
1:C:2408:ALA:HB2	1:C:2437:THR:HG22	1.64	0.78
1:D:3177:MSE:O	1:D:3181:VAL:HG23	1.84	0.78
1:E:4094:LYS:HD3	1:E:4560:SER:O	1.84	0.78
1:G:6103:ASP:HB3	1:G:6107:LEU:CD2	2.13	0.78
1:B:1109:PRO:HA	1:B:1113:THR:O	1.84	0.78
1:B:1166:ILE:HD13	1:B:1256:ASP:HB3	1.64	0.78
1:F:5122:GLN:O	1:F:5126:ILE:HG12	1.84	0.78
1:G:6268:LYS:HG2	1:G:6269:TYR:CE2	2.19	0.78
1:H:7498:LEU:O	1:H:7501:GLN:HB2	1.83	0.78
1:B:1283:THR:O	1:B:1286:VAL:HG23	1.84	0.78
1:C:2067:ARG:HB2	1:D:3217:PHE:HE1	1.49	0.78
1:F:5269:TYR:HB3	1:F:5273:TYR:CD1	2.18	0.78
1:A:350:LEU:HD22	1:A:354:ARG:NH1	1.99	0.78
1:B:1527:ALA:O	1:B:1531:THR:HG23	1.84	0.78
1:F:5320:ALA:O	1:F:5323:ILE:HB	1.84	0.78
1:B:1269:TYR:HB3	1:B:1273:TYR:HD1	1.49	0.77
1:C:2038:MSE:HB2	1:C:2059:GLU:HG3	1.64	0.77
1:F:5194:ARG:HH21	1:F:5197:ARG:HE	1.29	0.77
1:E:4061:GLN:HA	1:E:4064:GLN:NE2	1.98	0.77
1:E:4210:ILE:HG22	1:E:4214:LYS:HD2	1.66	0.77
1:G:6144:ARG:HH12	1:G:6244:ASP:HB3	1.44	0.77
1:A:454:LEU:HD13	1:A:458:ARG:HH11	1.46	0.77
1:B:1302:ILE:HA	1:B:1305:HIS:ND1	2.00	0.77
1:C:2339:LYS:HA	1:C:2367:HIS:CE1	2.19	0.77
1:D:3183:LYS:HG2	1:D:3187:TYR:HE1	1.49	0.77
1:H:7325:MSE:HE2	1:H:7492:LEU:HD13	1.66	0.77
1:B:1419:LEU:H	1:B:1419:LEU:HD22	1.50	0.77
1:C:2358:ILE:HG22	1:C:2362:GLN:HB3	1.65	0.77
1:E:4024:LYS:HA	1:E:4028:LEU:HD22	1.65	0.77
1:E:4354:ARG:HG3	1:E:4358:ILE:HD11	1.67	0.77
1:F:5432:GLU:O	1:F:5436:LEU:HB2	1.85	0.77
1:G:6205:VAL:CG1	1:G:6226:ASP:HB3	2.14	0.77
1:G:6210:ILE:HA	1:G:6213:LEU:HD12	1.64	0.77
1:G:6351:VAL:HG21	1:G:6369:ALA:HA	1.67	0.77
1:H:7548:ASP:OD2	1:H:7551:LYS:HB2	1.85	0.77
1:B:1376:THR:HG22	1:B:1379:ASP:H	1.48	0.77
1:C:2376:THR:HG22	1:C:2378:GLU:H	1.49	0.77
1:E:4177:MSE:HE2	1:E:4181:VAL:HG22	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1360:SER:O	1:B:1363:GLU:HG2	1.85	0.77
1:C:2030:LEU:HD13	1:D:3030:LEU:O	1.84	0.77
1:E:4382:ASN:O	1:E:4385:LYS:HD3	1.85	0.77
1:H:7325:MSE:HB3	1:H:7492:LEU:HD13	1.64	0.77
1:B:1166:ILE:HD13	1:B:1256:ASP:CB	2.15	0.77
1:C:2416:ILE:HD13	1:C:2442:LEU:O	1.85	0.77
1:C:2294:ALA:O	1:C:2297:VAL:HG22	1.85	0.76
1:D:3072:LEU:HA	1:D:3075:MSE:HE3	1.67	0.76
1:C:2088:ILE:O	1:C:2096:PHE:HB2	1.85	0.76
1:D:3351:VAL:HG21	1:D:3369:ALA:HA	1.66	0.76
1:F:5453:LYS:HA	1:F:5458:ARG:O	1.86	0.76
1:G:6025:GLY:O	1:G:6028:LEU:HB2	1.86	0.76
1:B:1310:LEU:HD21	1:B:1398:LEU:HB2	1.66	0.76
1:D:3243:THR:HB	1:D:3248:ARG:CD	2.15	0.76
1:B:1138:SER:HB3	1:C:2572:TRP:CE2	2.21	0.76
1:D:3205:VAL:O	1:D:3225:ARG:HA	1.85	0.76
1:A:283:THR:O	1:A:286:VAL:HG23	1.86	0.76
1:D:3061:GLN:CA	1:D:3064:GLN:HE21	1.92	0.76
1:D:3378:GLU:HG3	1:D:3379:ASP:H	1.50	0.76
1:E:4225:ARG:HH11	1:E:4225:ARG:HG2	1.51	0.76
1:G:6379:ASP:O	1:G:6383:ILE:HG13	1.86	0.76
1:G:6488:ASP:HA	1:G:6491:PHE:HD1	1.50	0.76
1:H:7343:MSE:HB3	1:H:7350:LEU:HD23	1.66	0.76
1:A:210:ILE:HG22	1:A:214:LYS:HD2	1.67	0.76
1:D:3529:LYS:O	1:D:3532:GLU:HG3	1.86	0.76
1:G:6490:VAL:HG22	1:G:6533:TYR:CE2	2.19	0.76
1:F:5072:LEU:HD11	1:F:5081:LYS:HB3	1.65	0.76
1:H:7550:ALA:O	1:H:7554:LYS:HG3	1.86	0.76
1:A:267:ARG:HH11	1:A:267:ARG:HG3	1.49	0.76
1:C:2061:GLN:HA	1:C:2064:GLN:HE21	1.50	0.76
1:C:2123:TYR:CD2	1:C:2219:MSE:HE1	2.20	0.76
1:D:3453:LYS:HD3	1:D:3457:GLY:HA2	1.68	0.76
1:F:5354:ARG:NE	1:F:5356:ALA:HB3	2.01	0.76
1:C:2453:LYS:HB2	1:C:2459:VAL:HG12	1.66	0.76
1:D:3253:GLN:HE22	1:D:3255:GLU:CG	1.96	0.76
1:G:6124:GLY:O	1:G:6217:PHE:HB3	1.86	0.76
1:H:7378:GLU:HB2	1:H:7403:VAL:HG23	1.68	0.76
1:C:2526:ILE:O	1:C:2530:VAL:HG23	1.85	0.75
1:H:7104:ILE:O	1:H:7108:MSE:HE2	1.86	0.75
1:D:3100:LEU:HD11	1:D:3111:VAL:HG21	1.66	0.75
1:E:4188:THR:HG21	1:E:4195:PRO:HG3	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:4349:LEU:HD21	1:E:4351:VAL:HG23	1.69	0.75
1:F:5057:LYS:HE3	1:F:5059:GLU:HG3	1.66	0.75
1:G:6324:VAL:HA	1:G:6327:MSE:HE3	1.69	0.75
1:B:1454:LEU:HD11	1:B:1460:PHE:CE2	2.21	0.75
1:H:7276:PHE:HB2	1:H:7281:GLN:OE1	1.85	0.75
1:A:261:ASN:HD22	1:A:261:ASN:H	1.30	0.75
1:B:1243:THR:HA	1:B:1247:GLY:O	1.87	0.75
1:H:7416:ILE:HD13	1:H:7416:ILE:H	1.51	0.75
1:A:188:THR:HG23	1:A:193:ILE:O	1.86	0.75
1:B:1413:ARG:HH21	1:B:1440:ARG:C	1.90	0.75
1:E:4530:VAL:HG12	1:E:4534:LEU:HD11	1.67	0.75
1:F:5310:LEU:HG	1:F:5393:ALA:HB2	1.66	0.75
1:D:3376:THR:CG2	1:D:3378:GLU:HG2	2.17	0.75
1:F:5302:ILE:O	1:F:5304:GLU:N	2.20	0.75
1:F:5419:LEU:H	1:F:5419:LEU:HD22	1.52	0.75
1:H:7302:ILE:HA	1:H:7305:HIS:CE1	2.21	0.75
1:H:7548:ASP:CG	1:H:7551:LYS:HB2	2.06	0.75
1:H:7559:ARG:HG3	1:H:7561:GLU:HG2	1.68	0.75
1:C:2041:THR:OG1	1:C:2044:GLU:HG3	1.87	0.75
1:D:3482:ASN:HD22	1:D:3482:ASN:N	1.84	0.75
1:E:4284:ALA:HB1	1:E:4322:LEU:HD13	1.68	0.74
1:G:6194:ARG:HB2	1:G:6197:ARG:HG3	1.67	0.74
1:G:6219:MSE:HG2	1:H:7038:MSE:HE1	1.68	0.74
1:A:526:ILE:O	1:A:530:VAL:HG23	1.87	0.74
1:B:1511:ARG:HH11	1:B:1511:ARG:CB	2.00	0.74
1:G:6240:LYS:HG3	1:G:6248:ARG:NH2	2.01	0.74
1:G:6314:GLU:HG3	1:G:6315:ALA:N	1.99	0.74
1:C:2270:ARG:HG3	1:C:2271:GLU:N	2.02	0.74
1:D:3150:TRP:NE1	1:D:3152:GLU:HB2	2.03	0.74
1:F:5378:GLU:O	1:F:5381:VAL:HB	1.86	0.74
1:H:7343:MSE:O	1:H:7350:LEU:HB2	1.87	0.74
1:A:391:GLY:HA3	1:A:427:GLU:HG2	1.70	0.74
1:A:60:THR:O	1:A:64:GLN:HG3	1.88	0.74
1:C:2412:GLU:O	1:C:2413:ARG:HG2	1.86	0.74
1:C:2422:PRO:C	1:C:2424:ALA:H	1.89	0.74
1:E:4059:GLU:HG2	1:E:4063:ILE:HG21	1.70	0.74
1:F:5160:VAL:HG13	1:F:5201:VAL:HB	1.68	0.74
1:G:6128:ARG:HH11	1:G:6128:ARG:HG2	1.51	0.74
1:G:6471:PHE:CG	1:G:6472:PRO:HD3	2.22	0.74
1:D:3437:THR:O	1:D:3440:ARG:HB2	1.87	0.74
1:G:6376:THR:HB	1:G:6379:ASP:OD1	1.88	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:5377:PHE:CZ	1:F:5389:ILE:HD11	2.22	0.74
1:G:6288:LEU:O	1:G:6292:LEU:HG	1.88	0.74
1:G:6413:ARG:HH21	1:G:6440:ARG:C	1.91	0.74
1:G:6466:ASN:HB3	1:G:6468:VAL:HG12	1.69	0.74
1:C:2559:ARG:HG3	1:C:2561:GLU:OE2	1.88	0.74
1:D:3150:TRP:CD1	1:D:3152:GLU:HB2	2.22	0.74
1:F:5097:TYR:O	1:F:5101:GLN:HG3	1.87	0.74
1:H:7351:VAL:O	1:H:7354:ARG:HB3	1.88	0.74
1:D:3144:ARG:HH11	1:D:3244:ASP:HB3	1.53	0.74
1:E:4505:GLU:O	1:E:4509:GLN:HG3	1.87	0.74
1:G:6164:GLU:HG3	1:G:6225:ARG:NH1	2.03	0.74
1:A:325:MSE:HE2	1:A:492:LEU:HD13	1.70	0.73
1:B:1454:LEU:HD11	1:B:1460:PHE:HE2	1.53	0.73
1:E:4416:ILE:HG12	1:E:4443:PHE:HD1	1.51	0.73
1:F:5389:ILE:HG22	1:F:5416:ILE:HA	1.67	0.73
1:F:5437:THR:O	1:F:5440:ARG:HB2	1.87	0.73
1:H:7086:MSE:HE1	1:H:7111:VAL:HG22	1.69	0.73
1:A:128:ARG:HH11	1:A:128:ARG:CG	2.00	0.73
1:A:302:ILE:HA	1:A:305:HIS:ND1	2.03	0.73
1:B:1259:ASN:O	1:B:1262:ALA:N	2.21	0.73
1:D:3210:ILE:HB	1:D:3214:LYS:HZ2	1.52	0.73
1:E:4400:THR:HG23	1:E:4403:VAL:CG2	2.18	0.73
1:F:5392:VAL:HG12	1:F:5392:VAL:O	1.89	0.73
1:G:6480:LEU:CD2	1:G:6556:ARG:HD3	2.18	0.73
1:D:3297:VAL:HG22	1:D:3298:ILE:HD13	1.70	0.73
1:D:3327:MSE:HE3	1:D:3337:ALA:HB1	1.69	0.73
1:E:4266:LEU:O	1:E:4270:ARG:HB3	1.87	0.73
1:G:6095:LEU:HG	1:G:6099:ILE:HD13	1.70	0.73
1:H:7408:ALA:CB	1:H:7437:THR:HG22	2.18	0.73
1:B:1391:GLY:HA3	1:B:1427:GLU:HG2	1.69	0.73
1:E:4231:TYR:O	1:E:4235:ILE:HG12	1.89	0.73
1:F:5128:ARG:CG	1:F:5128:ARG:HH11	2.00	0.73
1:F:5377:PHE:HZ	1:F:5389:ILE:HD11	1.52	0.73
1:F:5506:GLU:HA	1:F:5509:GLN:HG3	1.69	0.73
1:A:128:ARG:HG2	1:A:128:ARG:NH1	1.95	0.73
1:D:3188:THR:HG21	1:D:3195:PRO:HG3	1.70	0.73
1:D:3377:PHE:CZ	1:D:3389:ILE:HD11	2.24	0.73
1:B:1312:ALA:HB1	1:B:1343:MSE:HE3	1.71	0.73
1:C:2499:THR:C	1:C:2501:GLN:H	1.92	0.73
1:H:7171:ASP:O	1:H:7172:LEU:HD23	1.89	0.73
1:H:7522:VAL:O	1:H:7526:ILE:HG12	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1454:LEU:HD12	1:B:1458:ARG:HB2	1.69	0.73
1:D:3281:GLN:HB3	1:D:3491:PHE:CE2	2.23	0.73
1:E:4283:THR:O	1:E:4286:VAL:HG23	1.88	0.73
1:G:6481:CYS:SG	1:G:6531:THR:HB	2.27	0.73
1:A:512:LEU:HD12	1:A:512:LEU:H	1.52	0.73
1:B:1358:ILE:N	1:B:1358:ILE:HD12	2.04	0.73
1:E:4206:GLY:CA	1:E:4223:GLN:HE21	2.02	0.73
1:E:4258:GLY:O	1:E:4260:HIS:N	2.22	0.73
1:F:5306:LYS:HD2	1:F:5384:LEU:O	1.88	0.73
1:E:4315:ALA:HB3	1:E:4392:VAL:HG11	1.71	0.73
1:F:5298:ILE:HD11	1:F:5442:LEU:HD11	1.71	0.73
1:B:1380:ALA:O	1:B:1384:LEU:HB2	1.89	0.73
1:F:5266:LEU:O	1:F:5270:ARG:HB3	1.88	0.73
1:A:319:ILE:O	1:A:322:LEU:N	2.21	0.72
1:E:4177:MSE:CE	1:E:4200:PRO:HB2	2.15	0.72
1:A:253:GLN:NE2	1:A:278:ASP:HB2	2.04	0.72
1:A:397:ARG:NH2	1:A:429:THR:HG22	2.04	0.72
1:D:3310:LEU:HD21	1:D:3398:LEU:HB3	1.72	0.72
1:G:6204:ASP:OD1	1:G:6221:LEU:HB2	1.89	0.72
1:G:6300:LYS:HD2	1:G:6304:GLU:CD	2.10	0.72
1:G:6308:LEU:HD12	1:G:6309:PHE:N	2.04	0.72
1:H:7049:GLY:O	1:H:7050:LEU:HD23	1.88	0.72
1:A:404:ILE:HD13	1:A:432:GLU:O	1.90	0.72
1:A:453:LYS:HD3	1:A:457:GLY:HA2	1.71	0.72
1:C:2309:PHE:HB2	1:C:2343:MSE:HG3	1.70	0.72
1:D:3261:ASN:ND2	1:D:3261:ASN:H	1.84	0.72
1:D:3387:SER:HA	1:D:3411:ASN:OD1	1.89	0.72
1:H:7099:ILE:HA	1:H:7102:ASP:HB2	1.71	0.72
1:B:1295:GLN:HA	1:B:1298:ILE:HB	1.71	0.72
1:D:3352:LYS:HB2	1:D:3368:SER:HA	1.71	0.72
1:F:5196:ASP:OD1	1:F:5196:ASP:N	2.20	0.72
1:D:3041:THR:CG2	1:D:3044:GLU:HG3	2.18	0.72
1:H:7244:ASP:N	1:H:7248:ARG:NH1	2.37	0.72
1:E:4278:ASP:OD1	1:E:4282:GLY:HA3	1.89	0.72
1:H:7308:LEU:HD12	1:H:7309:PHE:H	1.54	0.72
1:B:1526:ILE:O	1:B:1530:VAL:HG23	1.88	0.72
1:C:2430:ALA:O	1:C:2433:ALA:HB3	1.88	0.72
1:D:3155:VAL:HB	1:D:3246:TYR:CD2	2.23	0.72
1:E:4396:GLY:O	1:E:4427:GLU:HA	1.90	0.72
1:F:5043:GLN:HG2	1:F:5566:LEU:HD11	1.72	0.72
1:G:6401:PRO:HA	1:G:6404:ILE:HD12	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1177:MSE:HE2	1:B:1181:VAL:HG23	1.72	0.72
1:D:3402:ASP:O	1:D:3405:ARG:HG2	1.88	0.72
1:F:5177:MSE:HE1	1:F:5200:PRO:CB	2.19	0.72
1:F:5528:ILE:O	1:F:5532:GLU:HG3	1.89	0.72
1:G:6479:ILE:HG22	1:G:6480:LEU:N	2.04	0.72
1:E:4312:ALA:HB1	1:E:4343:MSE:HE3	1.72	0.72
1:A:564:SER:C	1:A:565:LEU:HD23	2.10	0.71
1:F:5437:THR:HG21	1:F:5441:CYS:HB3	1.70	0.71
1:E:4041:THR:HG23	1:E:4044:GLU:HG3	1.70	0.71
1:A:137:ILE:HD11	1:A:230:GLN:HE21	1.55	0.71
1:B:1281:GLN:HB3	1:B:1491:PHE:CE2	2.25	0.71
1:E:4498:LEU:O	1:E:4501:GLN:HB2	1.91	0.71
1:F:5376:THR:HG22	1:F:5378:GLU:H	1.55	0.71
1:F:5408:ALA:HB2	1:F:5437:THR:HG22	1.71	0.71
1:C:2261:ASN:HD22	1:C:2261:ASN:N	1.87	0.71
1:E:4174:VAL:HG21	1:E:4219:MSE:O	1.91	0.71
1:G:6376:THR:O	1:G:6379:ASP:HB2	1.91	0.71
1:F:5352:LYS:HG2	1:F:5367:HIS:C	2.10	0.71
1:F:5506:GLU:HG2	1:F:5511:ARG:HD2	1.72	0.71
1:F:5527:ALA:O	1:F:5531:THR:HG23	1.90	0.71
1:A:377:PHE:HZ	1:A:389:ILE:HD11	1.55	0.71
1:B:1177:MSE:CE	1:B:1200:PRO:HB2	2.20	0.71
1:C:2155:VAL:O	1:C:2156:LYS:HE2	1.90	0.71
1:G:6454:LEU:HD11	1:G:6460:PHE:HE2	1.53	0.71
1:H:7354:ARG:NE	1:H:7356:ALA:HB3	2.06	0.71
1:A:290:GLY:HA2	4:A:8037:HOH:O	1.91	0.71
1:A:370:PRO:O	1:A:371:GLU:C	2.27	0.71
1:B:1042:LEU:HD21	1:D:3572:TRP:HB2	1.73	0.71
1:B:1394:GLY:HA2	1:B:1420:SER:HB3	1.73	0.71
1:G:6531:THR:HA	1:G:6534:LEU:HD12	1.73	0.71
1:H:7381:VAL:HG13	1:H:7407:MSE:HE1	1.73	0.71
1:B:1412:GLU:O	1:B:1440:ARG:HD2	1.91	0.71
1:C:2370:PRO:HD2	1:C:2373:ILE:HD11	1.73	0.71
1:C:2308:LEU:HB3	1:C:2389:ILE:CD1	2.21	0.71
1:D:3229:GLN:HG3	1:D:3233:ASP:OD1	1.90	0.71
1:G:6267:ARG:NH1	1:G:6267:ARG:HG3	2.02	0.71
1:G:6320:ALA:HA	1:G:6323:ILE:HD12	1.72	0.71
1:C:2128:ARG:NH1	1:C:2128:ARG:HG2	1.96	0.71
1:C:2030:LEU:HB3	1:D:3030:LEU:HD12	1.72	0.71
1:E:4059:GLU:HG2	1:E:4063:ILE:CG2	2.21	0.71
1:E:4086:MSE:O	1:E:4089:GLN:HB3	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:6271:GLU:O	1:G:6485:HIS:NE2	2.24	0.71
1:D:3143:VAL:HG11	1:D:3238:PHE:HA	1.72	0.70
1:F:5397:ARG:HA	1:F:5427:GLU:O	1.91	0.70
1:G:6207:THR:O	1:G:6224:LYS:HA	1.91	0.70
1:G:6416:ILE:HD13	1:G:6416:ILE:N	2.05	0.70
1:B:1326:SER:O	1:B:1329:GLU:HB3	1.90	0.70
1:C:2377:PHE:HZ	1:C:2389:ILE:CG1	2.04	0.70
1:D:3132:GLY:HA3	1:D:3200:PRO:HG2	1.72	0.70
1:E:4535:TYR:HE1	1:E:4546:PRO:HD2	1.54	0.70
1:H:7162:ASP:O	1:H:7225:ARG:NH2	2.24	0.70
1:H:7399:PHE:HB2	1:H:7428:CYS:HB3	1.73	0.70
1:A:51:GLN:NE2	1:A:51:GLN:HA	2.06	0.70
1:B:1207:THR:HG23	1:B:1213:LEU:HD21	1.71	0.70
1:E:4294:ALA:O	1:E:4297:VAL:HG13	1.92	0.70
1:G:6308:LEU:HD12	1:G:6309:PHE:H	1.54	0.70
1:A:44:GLU:O	1:A:48:LEU:HB2	1.92	0.70
1:B:1376:THR:HB	1:B:1379:ASP:CG	2.12	0.70
1:D:3310:LEU:HD21	1:D:3398:LEU:CB	2.22	0.70
1:E:4312:ALA:CB	1:E:4343:MSE:HE3	2.21	0.70
1:E:4317:LEU:H	1:E:4317:LEU:HD12	1.55	0.70
1:G:6143:VAL:O	1:G:6147:VAL:HG23	1.91	0.70
1:G:6413:ARG:HA	1:G:6440:ARG:O	1.91	0.70
1:H:7302:ILE:HA	1:H:7305:HIS:ND1	2.06	0.70
1:B:1480:LEU:HD23	1:B:1556:ARG:HD3	1.72	0.70
1:D:3137:ILE:HD11	1:D:3230:GLN:HB3	1.74	0.70
1:D:3268:LYS:O	4:D:8049:HOH:O	2.09	0.70
1:D:3535:TYR:CD2	1:D:3540:ALA:HB3	2.27	0.70
1:G:6182:GLY:HA2	1:G:6185:CYS:SG	2.32	0.70
1:B:1382:ASN:O	1:B:1385:LYS:HG3	1.91	0.70
1:D:3239:MSE:HE3	1:D:3273:TYR:CD1	2.26	0.70
1:G:6122:GLN:O	1:G:6126:ILE:HG12	1.92	0.70
1:B:1266:LEU:O	1:B:1270:ARG:HB3	1.92	0.70
1:B:1414:PRO:HD2	1:B:1441:CYS:HA	1.74	0.70
1:C:2370:PRO:HD2	1:C:2373:ILE:CD1	2.22	0.70
1:D:3071:ASN:HA	1:D:3074:LYS:HE3	1.74	0.70
1:D:3397:ARG:HA	1:D:3427:GLU:O	1.91	0.70
1:E:4512:LEU:H	1:E:4512:LEU:HD12	1.57	0.70
1:F:5169:LEU:N	1:F:5169:LEU:HD12	2.07	0.70
1:F:5357:LYS:C	1:F:5358:ILE:HD12	2.12	0.70
1:F:5416:ILE:HD13	1:F:5416:ILE:H	1.56	0.70
1:G:6395:ALA:HB3	1:G:6398:LEU:HD22	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1144:ARG:NH1	1:B:1244:ASP:HB3	2.06	0.70
1:D:3108:MSE:HB3	1:D:3109:PRO:HD3	1.74	0.70
1:D:3174:VAL:HG21	1:D:3219:MSE:O	1.92	0.70
1:E:4357:LYS:H	1:E:4357:LYS:NZ	1.90	0.70
1:G:6133:LEU:HD12	1:H:7052:GLY:O	1.91	0.70
1:A:295:GLN:HA	1:A:298:ILE:HB	1.74	0.70
1:A:332:LEU:HG	1:A:336:GLU:OE2	1.91	0.70
1:D:3327:MSE:HE2	1:D:3341:ILE:HD11	1.74	0.70
1:E:4402:ASP:HA	1:E:4405:ARG:HG2	1.74	0.70
1:D:3127:PHE:O	1:D:3128:ARG:HD3	1.91	0.70
1:F:5210:ILE:O	1:F:5214:LYS:HG2	1.92	0.70
1:H:7470:ILE:N	1:H:7470:ILE:HD12	2.07	0.70
1:A:112:TYR:CD2	1:A:113:THR:HG23	2.27	0.69
1:F:5333:SER:HB3	1:F:5336:GLU:OE1	1.91	0.69
1:F:5454:LEU:HD13	1:F:5458:ARG:NH1	2.07	0.69
1:A:293:ALA:HB3	1:A:512:LEU:HB3	1.73	0.69
1:A:309:PHE:HD1	1:A:390:ILE:HB	1.57	0.69
1:C:2260:HIS:O	1:C:2264:ARG:HG2	1.91	0.69
1:C:2376:THR:H	1:C:2379:ASP:HB2	1.56	0.69
1:E:4394:GLY:HA2	1:E:4420:SER:HB3	1.74	0.69
1:G:6467:ASN:C	1:G:6469:TYR:H	1.94	0.69
1:A:397:ARG:HH11	1:A:397:ARG:HG2	1.58	0.69
1:C:2172:LEU:O	1:C:2175:TYR:HB2	1.92	0.69
1:D:3374:PRO:CD	1:D:3383:ILE:HD12	2.19	0.69
1:E:4338:GLN:NE2	1:E:4364:PRO:HB3	2.07	0.69
1:G:6238:PHE:O	1:G:6242:ILE:HG12	1.91	0.69
1:G:6389:ILE:HG22	1:G:6416:ILE:HG22	1.72	0.69
1:H:7215:ASP:OD1	1:H:7216:PRO:HD2	1.92	0.69
1:B:1045:ARG:CZ	1:B:1058:ILE:HD13	2.22	0.69
1:F:5396:GLY:O	1:F:5427:GLU:HA	1.91	0.69
1:H:7261:ASN:N	1:H:7261:ASN:HD22	1.89	0.69
1:H:7378:GLU:O	1:H:7381:VAL:HB	1.91	0.69
1:A:488:ASP:HA	1:A:491:PHE:HD1	1.57	0.69
1:B:1379:ASP:O	1:B:1383:ILE:HG13	1.93	0.69
1:B:1476:LEU:O	1:B:1480:LEU:HD12	1.93	0.69
1:E:4240:LYS:HG3	1:E:4248:ARG:NH2	2.02	0.69
1:H:7269:TYR:HB3	1:H:7273:TYR:HD1	1.57	0.69
1:H:7377:PHE:CZ	1:H:7389:ILE:HD11	2.20	0.69
1:H:7422:PRO:O	1:H:7424:ALA:N	2.26	0.69
1:A:377:PHE:CZ	1:A:389:ILE:HD11	2.27	0.69
1:B:1232:ASP:HA	1:B:1235:ILE:HG12	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:4559:ARG:HG3	1:E:4561:GLU:OE2	1.92	0.69
1:F:5051:GLN:HE21	1:F:5051:GLN:HA	1.57	0.69
1:F:5357:LYS:HD3	1:F:5357:LYS:N	2.06	0.69
1:G:6298:ILE:HG22	1:G:6299:SER:N	2.06	0.69
1:B:1429:THR:HG23	1:B:1432:GLU:CG	2.21	0.69
1:C:2324:VAL:HA	1:C:2327:MSE:HE3	1.74	0.69
1:D:3394:GLY:O	1:D:3425:GLN:HG3	1.91	0.69
1:D:3518:ASN:O	1:D:3522:VAL:HG23	1.91	0.69
1:E:4352:LYS:HG3	1:E:4368:SER:HA	1.74	0.69
1:E:4339:LYS:HA	1:E:4367:HIS:NE2	2.07	0.69
1:F:5038:MSE:HE2	1:F:5055:PRO:HG2	1.73	0.69
1:F:5194:ARG:CB	1:F:5197:ARG:HG2	2.23	0.69
1:F:5414:PRO:HD2	1:F:5441:CYS:HA	1.74	0.69
1:G:6456:ASP:OD2	1:G:6458:ARG:HD3	1.92	0.69
1:H:7269:TYR:HA	1:H:7272:LYS:HB2	1.75	0.69
1:D:3162:ASP:O	1:D:3225:ARG:NH2	2.26	0.69
1:F:5432:GLU:HA	1:F:5436:LEU:HD13	1.75	0.69
1:C:2137:ILE:O	1:C:2140:ARG:HG2	1.92	0.69
1:F:5194:ARG:HH21	1:F:5197:ARG:NE	1.91	0.69
1:G:6381:VAL:HG13	1:G:6407:MSE:HE1	1.74	0.69
1:H:7466:ASN:HB3	1:H:7468:VAL:CG1	2.22	0.69
1:A:389:ILE:HG22	1:A:416:ILE:HA	1.73	0.69
1:B:1172:LEU:O	1:B:1175:TYR:HB2	1.92	0.69
1:D:3392:VAL:O	1:D:3392:VAL:HG12	1.91	0.69
1:E:4558:TRP:O	1:E:4559:ARG:HD3	1.93	0.69
1:F:5412:GLU:OE1	1:F:5412:GLU:HA	1.93	0.69
1:G:6075:MSE:HB3	1:G:6081:LYS:HE2	1.75	0.69
1:H:7407:MSE:HG3	1:H:7414:PRO:HB2	1.73	0.69
1:B:1351:VAL:O	1:B:1354:ARG:HG2	1.93	0.69
1:H:7470:ILE:N	1:H:7470:ILE:CD1	2.56	0.69
1:B:1435:THR:HG22	1:B:1454:LEU:HD23	1.73	0.68
1:D:3133:LEU:HB3	1:D:3201:VAL:HG13	1.76	0.68
1:G:6169:LEU:N	1:G:6169:LEU:HD12	2.08	0.68
1:A:342:TRP:CH2	1:A:367:HIS:HB2	2.28	0.68
1:B:1350:LEU:O	1:B:1366:THR:HA	1.92	0.68
1:C:2253:GLN:HG3	1:C:2276:PHE:CZ	2.28	0.68
1:F:5324:VAL:HA	1:F:5327:MSE:HE3	1.76	0.68
1:A:522:VAL:O	1:A:526:ILE:HG13	1.93	0.68
1:C:2376:THR:HG21	1:C:2378:GLU:OE2	1.94	0.68
1:E:4275:THR:OG1	1:E:4276:PHE:N	2.26	0.68
1:E:4320:ALA:HA	1:E:4323:ILE:HD12	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:6207:THR:HG23	1:G:6213:LEU:HD21	1.74	0.68
1:G:6312:ALA:HB1	1:G:6343:MSE:HE3	1.73	0.68
1:G:6289:ALA:CB	1:G:6498:LEU:HD23	2.23	0.68
1:B:1376:THR:HG22	1:B:1378:GLU:N	2.07	0.68
1:F:5466:ASN:HB3	1:F:5468:VAL:HG12	1.74	0.68
1:G:6166:ILE:HD13	1:G:6256:ASP:CG	2.14	0.68
1:A:414:PRO:HD2	1:A:440:ARG:O	1.93	0.68
1:B:1072:LEU:O	1:B:1075:MSE:HB2	1.94	0.68
1:B:1261:ASN:HD22	1:B:1261:ASN:H	1.36	0.68
1:C:2086:MSE:HE1	1:C:2111:VAL:HG13	1.76	0.68
1:C:2276:PHE:HB2	1:C:2281:GLN:OE1	1.93	0.68
1:C:2306:LYS:HD2	1:C:2385:LYS:O	1.92	0.68
1:D:3177:MSE:CE	1:D:3200:PRO:HB2	2.17	0.68
1:E:4350:LEU:HD13	1:E:4354:ARG:CZ	2.23	0.68
1:F:5477:ALA:HB1	1:F:5531:THR:HG22	1.76	0.68
1:G:6112:TYR:CD2	1:G:6113:THR:HG23	2.28	0.68
1:B:1174:VAL:HG23	1:B:1219:MSE:HE3	1.76	0.68
1:E:4075:MSE:HB3	1:E:4081:LYS:HD3	1.74	0.68
1:F:5188:THR:HG23	1:F:5193:ILE:O	1.94	0.68
1:G:6350:LEU:HD12	1:G:6366:THR:HG23	1.76	0.68
1:G:6480:LEU:HD22	1:G:6556:ARG:HD3	1.76	0.68
1:H:7553:VAL:O	1:H:7555:GLU:N	2.26	0.68
1:A:351:VAL:HG11	1:A:369:ALA:HB2	1.75	0.68
1:D:3537:ASN:N	1:D:3537:ASN:HD22	1.91	0.68
1:E:4109:PRO:HA	1:E:4113:THR:O	1.94	0.68
1:F:5177:MSE:CE	1:F:5200:PRO:HB2	2.22	0.68
1:G:6482:ASN:ND2	1:G:6542:ARG:HB2	2.07	0.68
1:A:276:PHE:HB3	1:A:486:ILE:HD12	1.76	0.68
1:B:1184:LEU:HD23	1:B:1200:PRO:HG3	1.74	0.68
1:B:1137:ILE:HA	1:B:1234:LEU:HD21	1.75	0.68
1:B:1437:THR:O	1:B:1440:ARG:HB2	1.94	0.68
1:D:3166:ILE:HG21	1:D:3172:LEU:HD12	1.76	0.68
1:F:5279:ASP:OD1	1:F:5279:ASP:N	2.23	0.68
1:B:1060:THR:O	1:B:1064:GLN:HG3	1.93	0.68
1:D:3199:LEU:HD12	1:D:3200:PRO:HD2	1.75	0.68
1:D:3308:LEU:HD13	1:D:3342:TRP:HB2	1.76	0.68
1:E:4527:ALA:O	1:E:4531:THR:HG23	1.93	0.68
1:G:6397:ARG:O	1:G:6398:LEU:HD12	1.94	0.68
1:G:6400:THR:HG23	1:G:6403:VAL:HG23	1.76	0.68
1:G:6456:ASP:OD1	1:G:6458:ARG:HB2	1.93	0.68
1:A:89:GLN:C	1:A:91:ARG:H	1.96	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1300:LYS:HG2	1:B:1304:GLU:OE1	1.94	0.68
1:E:4026:LYS:HG3	1:E:4029:MSE:HE3	1.75	0.68
1:A:502:LEU:HA	1:A:506:GLU:OE1	1.94	0.67
1:B:1443:PHE:O	1:B:1512:LEU:HD11	1.92	0.67
1:E:4357:LYS:H	1:E:4357:LYS:HZ3	1.42	0.67
1:G:6243:THR:HG22	1:G:6248:ARG:HA	1.75	0.67
1:G:6352:LYS:CG	1:G:6368:SER:HA	2.24	0.67
1:H:7481:CYS:SG	1:H:7534:LEU:HD12	2.33	0.67
1:A:535:TYR:OH	1:A:545:GLU:HA	1.94	0.67
1:B:1310:LEU:HD22	1:B:1399:PHE:CE2	2.30	0.67
1:D:3194:ARG:HB2	1:D:3197:ARG:CG	2.23	0.67
1:F:5470:ILE:HG22	1:F:5474:VAL:HG21	1.77	0.67
1:H:7144:ARG:NH1	1:H:7244:ASP:HB3	2.08	0.67
1:A:244:ASP:N	1:A:248:ARG:HH11	1.92	0.67
1:B:1339:LYS:HA	1:B:1367:HIS:CE1	2.29	0.67
1:B:1506:GLU:O	1:B:1511:ARG:HG2	1.93	0.67
1:C:2038:MSE:SE	1:C:2055:PRO:HG2	2.44	0.67
1:E:4215:ASP:OD1	1:E:4216:PRO:HD2	1.94	0.67
1:E:4384:LEU:O	1:E:4385:LYS:HB2	1.92	0.67
1:F:5339:LYS:HA	1:F:5367:HIS:NE2	2.09	0.67
1:G:6302:ILE:HG22	1:G:6340:LYS:NZ	2.09	0.67
1:H:7083:ILE:HD11	1:H:7126:ILE:CG2	2.24	0.67
1:C:2160:VAL:HG12	1:C:2201:VAL:HB	1.75	0.67
1:C:2188:THR:HG23	1:C:2193:ILE:O	1.93	0.67
1:C:2437:THR:O	1:C:2440:ARG:HB2	1.94	0.67
1:C:2480:LEU:HD22	1:C:2556:ARG:HD3	1.76	0.67
1:F:5174:VAL:HG21	1:F:5219:MSE:C	2.15	0.67
1:F:5306:LYS:HB3	1:F:5386:PRO:HA	1.76	0.67
1:G:6038:MSE:HE2	1:G:6057:LYS:O	1.94	0.67
1:G:6454:LEU:HD12	1:G:6458:ARG:CB	2.23	0.67
1:A:336:GLU:O	1:A:340:LYS:HD2	1.95	0.67
1:B:1350:LEU:HD22	1:B:1354:ARG:NH1	2.10	0.67
1:C:2030:LEU:HB3	1:D:3030:LEU:CD1	2.25	0.67
1:D:3377:PHE:HZ	1:D:3389:ILE:HD11	1.59	0.67
1:D:3429:THR:HG23	1:D:3432:GLU:OE1	1.93	0.67
1:A:86:MSE:HE2	1:A:86:MSE:HA	1.77	0.67
1:B:1302:ILE:HA	1:B:1305:HIS:HD1	1.60	0.67
1:B:1388:THR:HG23	1:B:1415:VAL:CB	2.22	0.67
1:B:1451:PRO:HG3	1:B:1461:THR:OG1	1.95	0.67
1:E:4177:MSE:HE3	1:E:4177:MSE:O	1.94	0.67
1:G:6269:TYR:HB3	1:G:6273:TYR:HD1	1.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:6217:PHE:HE1	1:H:7067:ARG:HB2	1.59	0.67
1:H:7524:ILE:O	1:H:7527:ALA:HB3	1.95	0.67
1:C:2104:ILE:CG1	1:C:2108:MSE:HE2	2.22	0.67
1:E:4164:GLU:HG3	1:E:4225:ARG:NH1	2.09	0.67
1:F:5526:ILE:O	1:F:5530:VAL:HG23	1.95	0.67
1:G:6437:THR:HG21	1:G:6441:CYS:HB3	1.75	0.67
1:G:6504:ASP:HA	1:G:6507:LEU:HD23	1.77	0.67
1:H:7394:GLY:O	1:H:7425:GLN:HG3	1.94	0.67
1:B:1482:ASN:N	1:B:1482:ASN:HD22	1.92	0.67
1:G:6169:LEU:H	1:G:6169:LEU:HD12	1.60	0.67
1:E:4392:VAL:HG12	1:E:4392:VAL:O	1.95	0.67
1:F:5454:LEU:HD13	1:F:5458:ARG:HH11	1.60	0.67
1:G:6255:GLU:O	1:G:6257:PHE:N	2.27	0.67
1:B:1179:ILE:HB	1:B:1180:PRO:HD3	1.76	0.67
1:C:2428:CYS:SG	1:C:2429:THR:N	2.68	0.67
1:D:3177:MSE:CE	1:D:3181:VAL:HG22	2.24	0.67
1:E:4103:ASP:OD2	1:E:4106:SER:HB2	1.93	0.67
1:F:5479:ILE:HG22	1:F:5480:LEU:N	2.10	0.67
1:G:6024:LYS:HA	1:G:6028:LEU:CD2	2.25	0.67
1:G:6351:VAL:CG2	1:G:6369:ALA:HA	2.25	0.67
1:H:7194:ARG:CB	1:H:7197:ARG:HG3	2.24	0.67
1:H:7229:GLN:O	1:H:7230:GLN:C	2.33	0.67
1:B:1505:GLU:O	1:B:1508:ALA:HB3	1.95	0.66
1:B:1537:ASN:HD22	1:B:1537:ASN:N	1.93	0.66
1:C:2307:ILE:HG13	1:C:2388:THR:CB	2.25	0.66
1:C:2407:MSE:HG3	1:C:2411:ASN:ND2	2.10	0.66
1:D:3045:ARG:NH1	1:D:3058:ILE:HD13	2.09	0.66
1:F:5377:PHE:O	1:F:5381:VAL:HG23	1.95	0.66
1:F:5431:GLU:O	1:F:5433:ALA:N	2.29	0.66
1:G:6177:MSE:O	1:G:6181:VAL:HG23	1.95	0.66
1:G:6302:ILE:HA	1:G:6305:HIS:CE1	2.30	0.66
1:H:7261:ASN:H	1:H:7261:ASN:HD22	1.40	0.66
1:H:7437:THR:O	1:H:7440:ARG:HB2	1.95	0.66
1:B:1505:GLU:CD	1:B:1505:GLU:H	1.99	0.66
1:D:3402:ASP:HA	1:D:3405:ARG:CD	2.25	0.66
1:E:4402:ASP:OD1	1:E:4402:ASP:N	2.28	0.66
1:F:5194:ARG:HB2	1:F:5197:ARG:CG	2.25	0.66
1:F:5469:TYR:C	1:F:5470:ILE:HD13	2.16	0.66
1:G:6374:PRO:HG3	1:G:6380:ALA:HA	1.76	0.66
1:A:341:ILE:O	1:A:367:HIS:NE2	2.28	0.66
1:C:2179:ILE:HB	1:C:2180:PRO:HD3	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2504:ASP:O	1:C:2507:LEU:HB2	1.94	0.66
1:G:6127:PHE:N	4:G:8062:HOH:O	2.24	0.66
1:G:6320:ALA:HB1	1:G:6365:PHE:CZ	2.29	0.66
1:A:300:LYS:HD2	1:A:304:GLU:OE1	1.95	0.66
1:B:1324:VAL:O	1:B:1328:VAL:HG23	1.95	0.66
1:B:1480:LEU:CD2	1:B:1556:ARG:HD3	2.25	0.66
1:C:2184:LEU:HD23	1:C:2200:PRO:HB3	1.75	0.66
1:D:3103:ASP:HB3	1:D:3107:LEU:HD22	1.76	0.66
1:E:4396:GLY:HA2	1:E:4425:GLN:HA	1.76	0.66
1:G:6041:THR:OG1	1:G:6044:GLU:HG3	1.95	0.66
1:G:6075:MSE:CG	1:G:6080:GLU:HG2	2.25	0.66
1:H:7120:CYS:O	1:H:7123:TYR:HB2	1.95	0.66
1:B:1466:ASN:O	1:B:1469:TYR:HD1	1.79	0.66
1:D:3452:VAL:O	1:D:3459:VAL:HA	1.96	0.66
1:F:5133:LEU:HB2	1:F:5199:LEU:HD11	1.77	0.66
1:F:5358:ILE:HG23	1:F:5362:GLN:HB3	1.78	0.66
1:G:6245:ARG:HG2	1:G:6246:TYR:CE1	2.30	0.66
1:G:6146:ILE:HG23	1:H:7052:GLY:HA3	1.76	0.66
1:H:7411:ASN:O	1:H:7414:PRO:HD3	1.96	0.66
1:A:196:ASP:OD1	1:A:196:ASP:N	2.24	0.66
1:H:7407:MSE:HG3	1:H:7414:PRO:CB	2.25	0.66
1:E:4172:LEU:O	1:E:4175:TYR:HB2	1.96	0.66
1:F:5393:ALA:HA	3:F:5601:NAD:O4B	1.95	0.66
1:A:352:LYS:HB2	1:A:368:SER:HA	1.78	0.66
1:A:401:PRO:HB3	1:A:436:LEU:HD21	1.78	0.66
1:B:1227:ARG:CG	1:B:1227:ARG:HH11	2.07	0.66
1:C:2227:ARG:HG2	1:C:2227:ARG:NH1	2.04	0.66
1:F:5410:ILE:HG22	1:F:5411:ASN:OD1	1.95	0.66
1:G:6416:ILE:HG12	1:G:6443:PHE:HD1	1.60	0.66
1:H:7196:ASP:N	1:H:7196:ASP:OD1	2.20	0.66
1:H:7408:ALA:HA	1:H:7414:PRO:HG3	1.77	0.66
1:H:7286:VAL:HG13	1:H:7470:ILE:HD13	1.77	0.66
1:A:419:LEU:HA	1:A:446:GLY:H	1.58	0.66
1:F:5269:TYR:HA	1:F:5272:LYS:HB2	1.78	0.66
1:F:5283:THR:O	1:F:5284:ALA:C	2.35	0.66
1:C:2376:THR:HG22	1:C:2378:GLU:N	2.11	0.66
1:D:3264:ARG:HG3	1:D:3265:PHE:N	2.11	0.66
1:D:3417:PHE:CD1	1:D:3444:ALA:HB3	2.30	0.66
1:D:3537:ASN:HB2	1:D:3539:MSE:HG3	1.76	0.66
1:E:4206:GLY:HA3	1:E:4223:GLN:HE21	1.61	0.66
1:F:5136:SER:OG	1:F:5221:LEU:HD21	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:7122:GLN:O	1:H:7125:HIS:HB2	1.96	0.66
1:B:1402:ASP:HA	1:B:1405:ARG:CD	2.24	0.65
1:D:3261:ASN:HA	1:D:3264:ARG:NE	2.10	0.65
1:D:3520:GLN:C	1:D:3524:ILE:HD12	2.17	0.65
1:E:4204:ASP:OD2	1:E:4221:LEU:HD22	1.96	0.65
1:E:4266:LEU:HD12	1:E:4266:LEU:O	1.96	0.65
1:F:5351:VAL:HG21	1:F:5369:ALA:HA	1.78	0.65
1:F:5381:VAL:HG13	1:F:5407:MSE:HE1	1.78	0.65
1:G:6123:TYR:CD2	1:G:6219:MSE:HE1	2.26	0.65
1:A:188:THR:HG21	1:A:195:PRO:HG3	1.77	0.65
1:B:1253:GLN:HE22	1:B:1255:GLU:HG2	1.62	0.65
1:D:3210:ILE:HB	1:D:3214:LYS:NZ	2.11	0.65
1:G:6079:LEU:HD11	1:G:6119:ALA:HA	1.79	0.65
1:G:6317:LEU:H	1:G:6317:LEU:CD1	2.01	0.65
1:H:7166:ILE:HG13	1:H:7172:LEU:HB2	1.78	0.65
1:H:7253:GLN:HG3	1:H:7276:PHE:CE2	2.32	0.65
1:A:253:GLN:HG3	1:A:276:PHE:CZ	2.32	0.65
1:B:1349:LEU:CD2	1:B:1351:VAL:HB	2.27	0.65
1:B:1392:VAL:O	1:B:1392:VAL:CG1	2.45	0.65
1:B:1535:TYR:CD2	1:B:1540:ALA:HB3	2.31	0.65
1:C:2392:VAL:O	1:C:2392:VAL:HG12	1.96	0.65
1:E:4261:ASN:HA	1:E:4264:ARG:HG2	1.77	0.65
1:E:4374:PRO:HB3	1:E:4383:ILE:HD12	1.77	0.65
1:C:2156:LYS:HB3	1:C:2479:ILE:HD13	1.78	0.65
1:D:3239:MSE:SE	1:D:3252:ILE:HD12	2.46	0.65
1:D:3378:GLU:HG3	1:D:3379:ASP:OD1	1.97	0.65
1:D:3430:ALA:HB2	1:D:3443:PHE:CE2	2.31	0.65
1:E:4352:LYS:HB2	1:E:4368:SER:HA	1.78	0.65
1:H:7085:ILE:HG23	1:H:7086:MSE:HE3	1.78	0.65
1:C:2432:GLU:CA	1:C:2436:LEU:HD13	2.26	0.65
1:C:2505:GLU:CD	1:C:2505:GLU:H	1.99	0.65
1:E:4437:THR:C	1:E:4439:GLY:H	1.98	0.65
1:F:5505:GLU:OE2	1:F:5505:GLU:N	2.28	0.65
1:G:6031:ASN:HB3	1:G:6034:THR:OG1	1.96	0.65
1:G:6358:ILE:HG21	1:G:6366:THR:OG1	1.97	0.65
1:H:7163:GLY:HA2	1:H:7166:ILE:HD11	1.77	0.65
1:A:323:ILE:HG22	1:A:327:MSE:HE2	1.77	0.65
1:A:408:ALA:HB2	1:A:437:THR:HG22	1.78	0.65
1:A:432:GLU:HA	1:A:436:LEU:HD13	1.78	0.65
1:B:1137:ILE:O	1:B:1140:ARG:HG2	1.96	0.65
1:E:4077:SER:HB3	1:E:4080:GLU:HB2	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:4295:GLN:HE22	1:E:4305:HIS:HE1	1.45	0.65
1:F:5333:SER:OG	1:F:5336:GLU:HG3	1.97	0.65
1:G:6163:GLY:O	1:G:6171:ASP:HA	1.96	0.65
1:H:7041:THR:HG23	1:H:7044:GLU:HG3	1.78	0.65
1:A:375:ASP:OD2	1:A:379:ASP:OD2	2.14	0.65
1:B:1240:LYS:HG3	1:B:1248:ARG:NH2	2.08	0.65
1:B:1243:THR:HG22	1:B:1248:ARG:HA	1.77	0.65
1:B:1408:ALA:HB2	1:B:1437:THR:HG22	1.78	0.65
1:B:1511:ARG:HH11	1:B:1511:ARG:HB3	1.61	0.65
1:D:3113:THR:HA	1:D:3116:VAL:HG12	1.78	0.65
1:E:4352:LYS:HG3	1:E:4368:SER:CA	2.27	0.65
1:E:4413:ARG:HA	1:E:4440:ARG:O	1.96	0.65
1:F:5512:LEU:HD12	1:F:5512:LEU:N	2.11	0.65
1:B:1261:ASN:N	1:B:1261:ASN:ND2	2.36	0.65
1:D:3043:GLN:HG2	1:D:3566:LEU:CD1	2.27	0.65
1:E:4184:LEU:O	1:E:4187:TYR:HB2	1.96	0.65
1:E:4350:LEU:HA	1:E:4354:ARG:HD3	1.78	0.65
1:F:5143:VAL:HG11	1:F:5238:PHE:HA	1.78	0.65
1:A:411:ASN:O	1:A:414:PRO:HD3	1.97	0.65
1:F:5429:THR:HG23	1:F:5432:GLU:CG	2.27	0.65
1:F:5503:THR:HG23	1:F:5506:GLU:CD	2.18	0.65
1:F:5559:ARG:HB3	1:F:5561:GLU:CG	2.26	0.65
1:G:6402:ASP:OD1	1:G:6402:ASP:N	2.29	0.65
1:H:7060:THR:OG1	1:H:7063:ILE:HG13	1.97	0.65
1:A:564:SER:O	1:A:565:LEU:HD23	1.97	0.65
1:B:1339:LYS:HA	1:B:1367:HIS:NE2	2.12	0.65
1:D:3317:LEU:H	1:D:3317:LEU:HD12	1.61	0.65
1:D:3360:SER:HA	1:D:3363:GLU:OE1	1.96	0.65
1:D:3386:PRO:HB2	1:D:3388:THR:O	1.97	0.65
1:E:4166:ILE:CG2	1:E:4172:LEU:HD12	2.27	0.65
1:E:4321:ASN:O	1:E:4324:VAL:HB	1.97	0.65
1:F:5351:VAL:CG2	1:F:5369:ALA:HA	2.27	0.65
1:D:3261:ASN:HA	1:D:3264:ARG:HG2	1.79	0.64
1:D:3350:LEU:HD22	1:D:3354:ARG:NH1	2.12	0.64
1:D:3531:THR:O	1:D:3534:LEU:HB2	1.97	0.64
1:F:5227:ARG:HH11	1:F:5227:ARG:HG2	1.62	0.64
1:F:5287:ALA:O	1:F:5290:GLY:N	2.29	0.64
1:F:5350:LEU:O	1:F:5366:THR:HA	1.97	0.64
1:F:5503:THR:HG23	1:F:5506:GLU:OE1	1.97	0.64
1:H:7106:SER:O	1:H:7109:PRO:HD2	1.96	0.64
1:A:264:ARG:HG3	1:A:265:PHE:N	2.12	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:471:PHE:CG	1:A:472:PRO:HD3	2.32	0.64
1:B:1487:SER:OG	1:B:1539:MSE:HE1	1.97	0.64
1:D:3374:PRO:HG3	1:D:3380:ALA:HA	1.79	0.64
1:E:4416:ILE:HD13	1:E:4442:LEU:O	1.98	0.64
1:F:5419:LEU:HA	1:F:5446:GLY:N	2.12	0.64
1:G:6268:LYS:HG2	1:G:6269:TYR:CD2	2.32	0.64
1:G:6191:ALA:HB1	1:G:6476:LEU:HD22	1.79	0.64
1:G:6482:ASN:HD22	1:G:6482:ASN:N	1.95	0.64
1:H:7150:TRP:CE3	1:H:7151:PRO:HD2	2.33	0.64
1:A:376:THR:HG22	1:A:378:GLU:N	2.11	0.64
1:B:1338:GLN:HA	1:B:1341:ILE:HG13	1.79	0.64
1:B:1352:LYS:N	1:B:1367:HIS:O	2.29	0.64
1:E:4303:SER:HA	1:E:4340:LYS:NZ	2.12	0.64
1:E:4191:ALA:HB2	1:E:4472:PRO:HB2	1.79	0.64
1:G:6327:MSE:CE	1:G:6341:ILE:HD11	2.21	0.64
1:H:7559:ARG:HG3	1:H:7561:GLU:CG	2.27	0.64
1:A:504:ASP:HA	1:A:507:LEU:HD23	1.80	0.64
1:C:2300:LYS:HG2	1:C:2304:GLU:OE2	1.98	0.64
1:C:2315:ALA:HB3	1:C:2392:VAL:CG1	2.27	0.64
1:C:2432:GLU:O	1:C:2436:LEU:HB2	1.97	0.64
1:C:2503:THR:OG1	1:C:2505:GLU:HG2	1.97	0.64
1:E:4261:ASN:HB3	1:E:4265:PHE:CE1	2.33	0.64
1:F:5113:THR:HA	1:F:5116:VAL:HG12	1.79	0.64
1:G:6492:LEU:HD23	1:G:6496:LYS:HD2	1.79	0.64
1:B:1335:GLN:C	1:B:1335:GLN:HE21	2.01	0.64
1:B:1406:ALA:O	1:B:1410:ILE:HG13	1.97	0.64
1:C:2098:ARG:HG3	1:C:2099:ILE:N	2.13	0.64
1:C:2136:SER:OG	1:C:2221:LEU:HD21	1.97	0.64
1:G:6126:ILE:O	1:G:6128:ARG:HD2	1.96	0.64
1:G:6160:VAL:CG1	1:G:6201:VAL:HB	2.24	0.64
1:H:7110:ILE:HG22	1:H:7111:VAL:N	2.12	0.64
1:H:7184:LEU:HG	1:H:7198:CYS:HB3	1.78	0.64
1:B:1291:LEU:HD23	1:B:1417:PHE:CZ	2.32	0.64
1:C:2569:VAL:CG1	1:C:2570:TYR:H	2.10	0.64
1:E:4535:TYR:CE1	1:E:4546:PRO:HD2	2.32	0.64
1:B:1320:ALA:HB1	1:B:1365:PHE:CE2	2.33	0.64
1:B:1453:LYS:HD3	1:B:1457:GLY:HA2	1.80	0.64
1:C:2067:ARG:HB2	1:D:3217:PHE:CE1	2.31	0.64
1:C:2101:GLN:O	1:C:2104:ILE:HG22	1.97	0.64
1:C:2308:LEU:HD12	1:C:2309:PHE:H	1.63	0.64
1:C:2422:PRO:O	1:C:2424:ALA:N	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3177:MSE:C	1:D:3180:PRO:HD2	2.17	0.64
1:F:5028:LEU:HD21	1:F:5048:LEU:HD12	1.79	0.64
1:F:5359:ASP:O	1:F:5362:GLN:HB2	1.98	0.64
1:F:5419:LEU:N	1:F:5419:LEU:HD13	2.11	0.64
1:G:6146:ILE:O	1:G:6149:ASN:HB2	1.97	0.64
1:H:7270:ARG:HG3	1:H:7271:GLU:N	2.13	0.64
1:H:7415:VAL:CG1	1:H:7442:LEU:HB2	2.22	0.64
1:A:42:LEU:O	1:A:46:GLN:HG3	1.98	0.64
1:C:2187:TYR:O	1:C:2191:ALA:HB3	1.98	0.64
1:F:5419:LEU:HA	1:F:5446:GLY:CA	2.27	0.64
1:G:6471:PHE:CD2	1:G:6472:PRO:HD3	2.33	0.64
1:B:1293:ALA:HB3	1:B:1512:LEU:HB3	1.78	0.64
1:C:2303:SER:HA	1:C:2340:LYS:NZ	2.13	0.64
1:C:2399:PHE:HB2	1:C:2428:CYS:HB3	1.79	0.64
1:E:4225:ARG:HH11	1:E:4225:ARG:CG	2.11	0.64
1:F:5079:LEU:HD13	1:F:5118:LEU:HD22	1.79	0.64
1:F:5197:ARG:HH11	1:F:5197:ARG:HG3	1.63	0.64
1:G:6113:THR:HA	1:G:6116:VAL:HG12	1.79	0.64
1:G:6210:ILE:HG22	1:G:6214:LYS:HE3	1.78	0.64
1:G:6298:ILE:HD11	1:G:6442:LEU:HD11	1.79	0.64
1:G:6468:VAL:HA	1:G:6471:PHE:CE2	2.33	0.64
1:G:6191:ALA:HB1	1:G:6476:LEU:CD2	2.28	0.64
1:H:7247:GLY:O	1:H:7250:THR:HB	1.98	0.64
1:H:7402:ASP:HA	1:H:7405:ARG:HD2	1.79	0.64
1:D:3095:LEU:O	1:D:3098:ARG:N	2.30	0.64
1:E:4522:VAL:O	1:E:4526:ILE:HG13	1.98	0.64
1:F:5211:ALA:O	1:F:5214:LYS:HG3	1.98	0.64
1:F:5423:THR:HG22	1:F:5423:THR:O	1.96	0.64
1:F:5419:LEU:HA	1:F:5446:GLY:HA3	1.80	0.64
1:A:432:GLU:O	1:A:436:LEU:HB2	1.98	0.63
1:D:3194:ARG:CB	1:D:3197:ARG:HG2	2.28	0.63
1:D:3482:ASN:H	1:D:3482:ASN:HD22	1.46	0.63
1:E:4264:ARG:HG3	1:E:4265:PHE:N	2.11	0.63
1:F:5179:ILE:HB	1:F:5180:PRO:CD	2.28	0.63
1:G:6027:PRO:HA	1:G:6030:LEU:HB2	1.80	0.63
1:G:6177:MSE:O	1:G:6180:PRO:HD2	1.98	0.63
1:H:7390:ILE:HG23	1:H:7417:PHE:HB2	1.79	0.63
1:A:255:GLU:O	1:A:257:PHE:HD1	1.82	0.63
1:B:1251:LEU:HD12	1:B:1252:ILE:N	2.12	0.63
1:C:2354:ARG:NE	1:C:2356:ALA:HB3	2.13	0.63
1:D:3302:ILE:HG22	1:D:3303:SER:N	2.12	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:6158:VAL:HA	1:G:6199:LEU:O	1.98	0.63
1:H:7415:VAL:HG13	1:H:7442:LEU:CB	2.19	0.63
1:B:1135:ILE:HG23	1:B:1143:VAL:HG22	1.80	0.63
1:B:1338:GLN:HG2	1:B:1339:LYS:N	2.13	0.63
1:B:1453:LYS:HG3	1:B:1459:VAL:HG13	1.80	0.63
1:E:4531:THR:CA	1:E:4534:LEU:HD12	2.28	0.63
1:G:6311:GLY:HA3	1:G:6392:VAL:O	1.99	0.63
1:H:7086:MSE:CA	1:H:7086:MSE:HE2	2.29	0.63
1:H:7243:THR:C	1:H:7248:ARG:HH11	2.02	0.63
1:H:7278:ASP:C	1:H:7280:ILE:H	2.01	0.63
1:H:7381:VAL:HG13	1:H:7407:MSE:CE	2.27	0.63
1:B:1258:GLY:O	1:B:1259:ASN:C	2.36	0.63
1:D:3315:ALA:HB3	1:D:3392:VAL:CG1	2.29	0.63
1:E:4293:ALA:O	1:E:4296:LYS:HB3	1.98	0.63
1:F:5100:LEU:HD11	1:F:5111:VAL:HG21	1.79	0.63
1:G:6342:TRP:CZ3	1:G:6349:LEU:HD21	2.33	0.63
1:B:1319:ILE:O	1:B:1323:ILE:HG13	1.99	0.63
1:B:1389:ILE:O	1:B:1390:ILE:HG13	1.98	0.63
1:B:1396:GLY:O	1:B:1427:GLU:HA	1.97	0.63
1:C:2258:GLY:O	1:C:2259:ASN:C	2.36	0.63
1:C:2398:LEU:HD12	1:C:2398:LEU:N	2.13	0.63
1:D:3400:THR:O	1:D:3404:ILE:HG13	1.99	0.63
1:E:4535:TYR:HD2	1:E:4540:ALA:HB3	1.61	0.63
1:F:5381:VAL:HG13	1:F:5407:MSE:CE	2.29	0.63
1:F:5471:PHE:CG	1:F:5472:PRO:HD3	2.34	0.63
1:A:498:LEU:O	1:A:501:GLN:HB2	1.99	0.63
1:B:1408:ALA:O	1:B:1440:ARG:NH2	2.20	0.63
1:E:4177:MSE:O	1:E:4180:PRO:HD2	1.99	0.63
1:E:4350:LEU:HD22	1:E:4354:ARG:HH12	1.59	0.63
1:E:4351:VAL:O	1:E:4354:ARG:HG2	1.98	0.63
1:F:5261:ASN:ND2	1:F:5261:ASN:H	1.96	0.63
1:G:6090:GLU:HG3	1:G:6131:LYS:HE2	1.80	0.63
1:G:6283:THR:O	1:G:6286:VAL:HG23	1.98	0.63
1:H:7194:ARG:HB2	1:H:7197:ARG:HG3	1.79	0.63
1:H:7416:ILE:N	1:H:7416:ILE:HD13	2.14	0.63
1:A:259:ASN:H	1:A:259:ASN:HD22	1.47	0.63
1:A:310:LEU:O	1:A:344:PHE:O	2.17	0.63
1:A:543:TYR:HB2	1:A:544:PRO:HA	1.79	0.63
1:E:4357:LYS:N	1:E:4357:LYS:NZ	2.47	0.63
1:F:5047:MSE:HE3	1:F:5566:LEU:HD22	1.80	0.63
1:G:6038:MSE:HE1	1:G:6057:LYS:HB3	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:6209:ASN:OD1	1:G:6211:ALA:HB3	1.98	0.63
1:G:6429:THR:HG23	1:G:6432:GLU:CD	2.19	0.63
1:H:7036:LYS:HE3	1:H:7039:ALA:O	1.98	0.63
1:H:7126:ILE:O	1:H:7128:ARG:HD2	1.98	0.63
1:H:7296:LYS:HE2	1:H:7507:LEU:HD21	1.79	0.63
1:H:7512:LEU:N	1:H:7512:LEU:HD12	2.14	0.63
1:A:535:TYR:CD1	1:A:549:LYS:HE3	2.33	0.63
1:B:1243:THR:HB	1:B:1248:ARG:HD2	1.79	0.63
1:B:1269:TYR:HB3	1:B:1273:TYR:CD1	2.31	0.63
1:C:2402:ASP:O	1:C:2405:ARG:HG2	1.99	0.63
1:C:2445:SER:O	1:C:2464:GLN:HA	1.98	0.63
1:G:6314:GLU:CG	1:G:6315:ALA:N	2.62	0.63
1:G:6319:ILE:O	1:G:6323:ILE:HG13	1.98	0.63
1:G:6551:LYS:O	1:G:6555:GLU:HB2	1.99	0.63
1:F:5572:TRP:CB	1:H:7042:LEU:HD21	2.23	0.63
1:A:550:ALA:O	1:A:554:LYS:HG3	1.99	0.63
1:B:1349:LEU:HD23	1:B:1351:VAL:HB	1.81	0.63
1:C:2072:LEU:HD11	1:C:2081:LYS:HB3	1.80	0.63
1:D:3293:ALA:O	1:D:3296:LYS:HB3	1.99	0.63
1:F:5041:THR:HG23	1:F:5044:GLU:HB2	1.80	0.63
1:F:5303:SER:HA	1:F:5340:LYS:NZ	2.13	0.63
1:G:6468:VAL:O	1:G:6519:ILE:HD11	1.98	0.63
1:G:6537:ASN:HB3	1:G:6539:MSE:SE	2.49	0.63
1:B:1347:TYR:HB3	1:B:1356:ALA:HB2	1.80	0.62
1:B:1392:VAL:O	1:B:1392:VAL:HG12	1.99	0.62
1:F:5521:GLU:HA	1:F:5524:ILE:HD12	1.79	0.62
1:F:5572:TRP:HB2	1:H:7042:LEU:CD2	2.27	0.62
1:G:6401:PRO:HG2	1:G:6402:ASP:OD1	1.98	0.62
1:H:7283:THR:O	1:H:7286:VAL:HG23	1.98	0.62
1:H:7325:MSE:HE1	1:H:7489:SER:CA	2.22	0.62
1:H:7470:ILE:HD11	1:H:7498:LEU:HD22	1.79	0.62
1:C:2308:LEU:HD12	1:C:2309:PHE:N	2.14	0.62
1:C:2352:LYS:CG	1:C:2368:SER:HA	2.29	0.62
1:F:5094:LYS:HD3	1:F:5560:SER:O	1.99	0.62
1:G:6153:ASN:O	1:G:6246:TYR:HE2	1.83	0.62
1:H:7116:VAL:HG13	1:H:7117:GLY:N	2.15	0.62
1:H:7261:ASN:HB3	1:H:7265:PHE:CE1	2.34	0.62
1:H:7396:GLY:O	1:H:7427:GLU:HA	1.99	0.62
1:H:7407:MSE:HA	1:H:7410:ILE:HD12	1.79	0.62
1:H:7422:PRO:C	1:H:7424:ALA:H	2.01	0.62
1:H:7493:GLU:HA	1:H:7496:LYS:HD2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:392:VAL:HG12	1:A:392:VAL:O	1.99	0.62
1:B:1116:VAL:HG13	1:B:1117:GLY:N	2.14	0.62
1:B:1238:PHE:CE1	1:B:1242:ILE:HG13	2.34	0.62
1:C:2376:THR:O	1:C:2379:ASP:HB2	1.99	0.62
1:C:2408:ALA:CB	1:C:2437:THR:HG22	2.28	0.62
1:C:2531:THR:HA	1:C:2534:LEU:HD12	1.81	0.62
1:E:4300:LYS:HE2	1:E:4304:GLU:CD	2.20	0.62
1:G:6300:LYS:HD2	1:G:6304:GLU:HB2	1.80	0.62
1:B:1135:ILE:O	1:B:1203:ILE:HG23	2.00	0.62
1:D:3106:SER:O	1:D:3109:PRO:HD2	1.99	0.62
1:D:3204:ASP:OD1	1:D:3221:LEU:HB2	2.00	0.62
1:F:5456:ASP:CB	1:F:5458:ARG:HD3	2.29	0.62
1:E:4569:VAL:HG21	1:G:6047:MSE:HE2	1.82	0.62
1:G:6185:CYS:O	1:G:6189:ALA:N	2.30	0.62
1:G:6533:TYR:O	1:G:6537:ASN:HB2	2.00	0.62
1:H:7042:LEU:HD12	1:H:7042:LEU:O	2.00	0.62
1:H:7086:MSE:CE	1:H:7086:MSE:CA	2.78	0.62
1:A:146:ILE:HD12	1:A:146:ILE:N	2.14	0.62
1:B:1113:THR:HA	1:B:1116:VAL:HG12	1.81	0.62
1:D:3179:ILE:HB	1:D:3180:PRO:HD3	1.81	0.62
1:D:3253:GLN:NE2	1:D:3254:PHE:O	2.32	0.62
1:G:6210:ILE:CA	1:G:6213:LEU:HD12	2.29	0.62
1:G:6492:LEU:O	1:G:6495:ALA:HB3	1.99	0.62
1:H:7271:GLU:O	1:H:7485:HIS:NE2	2.33	0.62
1:A:501:GLN:HA	1:A:501:GLN:NE2	2.15	0.62
1:D:3261:ASN:HB3	1:D:3265:PHE:CE1	2.35	0.62
1:D:3289:ALA:O	1:D:3499:THR:OG1	2.17	0.62
1:E:4123:TYR:HD2	1:E:4219:MSE:HE1	1.65	0.62
1:F:5551:LYS:O	1:F:5555:GLU:HB2	1.99	0.62
1:G:6140:ARG:NH1	1:G:6230:GLN:HG2	2.14	0.62
1:G:6177:MSE:HE1	1:G:6180:PRO:HB2	1.81	0.62
1:A:351:VAL:HG21	1:A:369:ALA:HA	1.82	0.62
1:A:566:LEU:CD2	1:A:567:PRO:HD2	2.29	0.62
1:C:2028:LEU:HD21	1:C:2048:LEU:HD12	1.81	0.62
1:D:3320:ALA:CA	1:D:3323:ILE:HD12	2.29	0.62
1:D:3291:LEU:HD23	1:D:3417:PHE:CE2	2.35	0.62
1:H:7179:ILE:HB	1:H:7180:PRO:CD	2.29	0.62
1:A:377:PHE:O	1:A:381:VAL:HG23	2.00	0.62
1:C:2303:SER:HA	1:C:2340:LYS:HZ1	1.63	0.62
1:C:2374:PRO:HD3	1:C:2383:ILE:HD12	1.81	0.62
1:D:3061:GLN:HG2	1:D:3098:ARG:HD3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3174:VAL:HG11	1:D:3220:GLY:HA3	1.80	0.62
1:E:4174:VAL:CG2	1:E:4219:MSE:HE3	2.26	0.62
1:G:6137:ILE:HG22	1:G:6221:LEU:CD2	2.29	0.62
1:G:6261:ASN:HB3	1:G:6265:PHE:CE1	2.35	0.62
1:G:6267:ARG:HH11	1:G:6267:ARG:CG	2.12	0.62
1:G:6288:LEU:O	1:G:6288:LEU:HG	1.98	0.62
1:G:6317:LEU:O	1:G:6320:ALA:HB3	1.99	0.62
1:H:7413:ARG:HA	1:H:7440:ARG:O	1.99	0.62
1:B:1137:ILE:HA	1:B:1234:LEU:CD2	2.29	0.62
1:C:2388:THR:HG23	1:C:2415:VAL:CB	2.30	0.62
1:D:3184:LEU:HA	1:D:3187:TYR:HB2	1.81	0.62
1:E:4099:ILE:O	1:E:4102:ASP:HB2	1.99	0.62
1:H:7396:GLY:HA2	1:H:7425:GLN:HA	1.80	0.62
1:H:7511:ARG:HH11	1:H:7511:ARG:CB	2.13	0.62
1:A:255:GLU:O	1:A:257:PHE:N	2.33	0.61
1:C:2261:ASN:H	1:C:2261:ASN:ND2	1.92	0.61
1:C:2259:ASN:O	1:C:2262:ALA:N	2.33	0.61
1:C:2432:GLU:O	1:C:2436:LEU:HD13	2.00	0.61
1:E:4350:LEU:HD13	1:E:4354:ARG:NE	2.15	0.61
1:F:5044:GLU:O	1:F:5048:LEU:HD23	2.00	0.61
1:F:5051:GLN:NE2	1:F:5051:GLN:HA	2.15	0.61
1:F:5453:LYS:CB	1:F:5459:VAL:HG13	2.24	0.61
1:F:5506:GLU:HG2	1:F:5511:ARG:CD	2.30	0.61
1:F:5537:ASN:HD22	1:F:5537:ASN:N	1.97	0.61
1:G:6294:ALA:O	1:G:6297:VAL:HG22	1.99	0.61
1:H:7308:LEU:HD12	1:H:7309:PHE:N	2.14	0.61
1:H:7487:SER:O	1:H:7490:VAL:HG23	2.00	0.61
1:A:157:ALA:O	1:A:198:CYS:HA	1.99	0.61
1:B:1027:PRO:HA	1:B:1030:LEU:HB2	1.81	0.61
1:C:2162:ASP:O	1:C:2225:ARG:NH2	2.28	0.61
1:C:2440:ARG:HH11	1:C:2440:ARG:HB3	1.65	0.61
1:E:4416:ILE:HD13	1:E:4416:ILE:H	1.64	0.61
1:B:1112:TYR:CD2	1:B:1113:THR:HG23	2.36	0.61
1:B:1405:ARG:O	1:B:1408:ALA:HB3	2.00	0.61
1:B:1525:ASN:HD22	1:B:1525:ASN:N	1.98	0.61
1:C:2469:TYR:CZ	1:C:2516:LEU:HD13	2.34	0.61
1:D:3120:CYS:SG	1:D:3179:ILE:HG12	2.40	0.61
1:E:4104:ILE:HG13	1:E:4108:MSE:HE2	1.81	0.61
1:E:4363:GLU:O	1:E:4366:THR:N	2.27	0.61
1:F:5451:PRO:HA	1:F:5460:PHE:O	2.01	0.61
1:G:6049:GLY:O	1:G:6050:LEU:HD23	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:6369:ALA:HB1	1:G:6373:ILE:CD1	2.30	0.61
1:G:6402:ASP:HA	1:G:6405:ARG:HD2	1.82	0.61
1:H:7184:LEU:HA	1:H:7187:TYR:HB2	1.82	0.61
1:A:137:ILE:HG13	1:A:137:ILE:O	2.00	0.61
1:B:1333:SER:OG	1:B:1336:GLU:HG3	2.01	0.61
1:D:3263:PHE:O	1:D:3266:LEU:HB3	2.01	0.61
1:H:7177:MSE:HE1	1:H:7200:PRO:CB	2.26	0.61
1:A:148:ASP:HA	1:A:245:ARG:HH11	1.64	0.61
1:B:1098:ARG:HG3	1:B:1099:ILE:N	2.14	0.61
1:E:4284:ALA:CB	1:E:4322:LEU:HD13	2.29	0.61
1:F:5253:GLN:HE22	1:F:5255:GLU:HG2	1.64	0.61
1:A:387:SER:O	1:A:415:VAL:HG23	2.00	0.61
1:B:1042:LEU:CD2	1:D:3572:TRP:HB2	2.30	0.61
1:F:5174:VAL:HG22	1:F:5218:TYR:CE2	2.36	0.61
1:H:7415:VAL:HG22	1:H:7442:LEU:CD1	2.30	0.61
1:B:1023:GLU:HA	1:B:1023:GLU:OE1	2.00	0.61
1:B:1310:LEU:HD22	1:B:1399:PHE:HE2	1.62	0.61
1:B:1443:PHE:CZ	1:B:1445:SER:HB3	2.36	0.61
1:B:1275:THR:O	1:B:1486:ILE:HD12	2.01	0.61
1:C:2093:GLU:OE1	1:C:2195:PRO:HB2	2.01	0.61
1:C:2376:THR:CG2	1:C:2378:GLU:HB3	2.30	0.61
1:D:3194:ARG:HB2	1:D:3197:ARG:HG2	1.83	0.61
1:D:3313:GLY:O	1:D:3315:ALA:N	2.34	0.61
1:E:4370:PRO:HD2	1:E:4373:ILE:HD11	1.82	0.61
1:F:5061:GLN:HG3	1:F:5562:TYR:CE1	2.35	0.61
1:G:6165:ARG:HB2	1:G:6257:PHE:O	2.00	0.61
1:H:7503:THR:O	1:H:7507:LEU:HD22	2.01	0.61
1:A:244:ASP:N	1:A:248:ARG:NH1	2.48	0.61
1:D:3183:LYS:HG2	1:D:3187:TYR:CE1	2.34	0.61
1:E:4174:VAL:HG11	1:E:4220:GLY:HA3	1.83	0.61
1:E:4332:LEU:HD21	1:E:4340:LYS:HD2	1.83	0.61
1:F:5124:GLY:O	1:F:5217:PHE:HB3	2.00	0.61
1:F:5376:THR:HG22	1:F:5378:GLU:N	2.16	0.61
1:F:5402:ASP:HA	1:F:5405:ARG:HG2	1.83	0.61
1:G:6401:PRO:HA	1:G:6436:LEU:CD2	2.31	0.61
1:G:6522:VAL:O	1:G:6526:ILE:HG12	2.01	0.61
1:H:7392:VAL:HG12	1:H:7392:VAL:O	2.01	0.61
1:A:79:LEU:O	1:A:79:LEU:HG	2.01	0.61
1:A:94:LYS:HD3	1:A:558:TRP:CZ2	2.35	0.61
1:B:1024:LYS:O	1:B:1027:PRO:HD2	2.01	0.61
1:E:4470:ILE:C	1:E:4472:PRO:HD2	2.21	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:5061:GLN:OE1	1:F:5098:ARG:HD3	2.01	0.61
1:F:5139:ASP:OD2	1:F:5146:ILE:HD11	2.01	0.61
1:G:6083:ILE:O	1:G:6083:ILE:HG22	2.01	0.61
1:G:6109:PRO:HA	1:G:6113:THR:O	2.01	0.61
1:G:6264:ARG:HG3	1:G:6265:PHE:N	2.15	0.61
1:H:7309:PHE:HB2	1:H:7343:MSE:HG3	1.82	0.61
1:A:407:MSE:HG3	1:A:414:PRO:CB	2.31	0.61
1:A:43:GLN:HG2	1:A:47:MSE:HE3	1.81	0.61
1:B:1334:GLU:O	1:B:1337:ALA:HB3	2.00	0.61
1:C:2065:ALA:O	1:C:2068:PHE:HB3	2.01	0.61
1:C:2352:LYS:HB2	1:C:2368:SER:HA	1.83	0.61
1:D:3199:LEU:HD12	1:D:3200:PRO:CD	2.30	0.61
1:E:4037:GLY:C	1:E:4039:ALA:H	2.04	0.61
1:E:4377:PHE:O	1:E:4381:VAL:HG23	2.01	0.61
1:F:5197:ARG:HG3	1:F:5197:ARG:NH1	2.16	0.61
1:G:6210:ILE:O	1:G:6214:LYS:HD2	2.01	0.61
1:H:7044:GLU:O	1:H:7048:LEU:HB2	2.01	0.61
1:A:261:ASN:N	1:A:261:ASN:HD22	1.98	0.60
1:A:487:SER:O	1:A:490:VAL:HG23	2.00	0.60
1:B:1210:ILE:O	1:B:1213:LEU:N	2.34	0.60
1:E:4300:LYS:HG2	1:E:4304:GLU:OE1	2.01	0.60
1:E:4512:LEU:HD12	1:E:4512:LEU:N	2.15	0.60
1:E:4571:GLU:HG3	1:E:4571:GLU:O	1.99	0.60
1:G:6219:MSE:CG	1:H:7038:MSE:HE1	2.31	0.60
1:G:6245:ARG:O	1:G:6245:ARG:HG3	2.00	0.60
1:G:6397:ARG:HA	1:G:6427:GLU:O	2.01	0.60
1:B:1354:ARG:HG3	1:B:1358:ILE:HD11	1.82	0.60
1:B:1359:ASP:OD2	1:B:1362:GLN:N	2.34	0.60
1:E:4307:ILE:HG13	1:E:4388:THR:HB	1.82	0.60
1:G:6100:LEU:HD23	1:G:6189:ALA:HB2	1.83	0.60
1:D:3169:LEU:HD12	1:D:3169:LEU:N	2.16	0.60
1:D:3188:THR:HG23	1:D:3193:ILE:O	2.00	0.60
1:F:5496:LYS:O	1:F:5500:SER:OG	2.18	0.60
1:H:7397:ARG:HA	1:H:7427:GLU:O	2.00	0.60
1:A:194:ARG:HB2	1:A:197:ARG:HG3	1.83	0.60
1:B:1104:ILE:HG13	1:B:1108:MSE:HE2	1.82	0.60
1:B:1232:ASP:N	1:B:1232:ASP:OD2	2.30	0.60
1:B:1297:VAL:HG23	1:B:1297:VAL:O	2.01	0.60
1:B:1354:ARG:NH2	1:B:1356:ALA:HB3	2.16	0.60
1:C:2498:LEU:O	1:C:2501:GLN:HB2	2.02	0.60
1:D:3345:ASP:HB2	3:D:3601:NAD:O2B	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3419:LEU:O	1:D:3446:GLY:HA3	2.01	0.60
1:F:5276:PHE:C	1:F:5276:PHE:CD1	2.74	0.60
1:F:5543:TYR:HB2	1:F:5544:PRO:HA	1.83	0.60
1:G:6038:MSE:CE	1:G:6055:PRO:HG2	2.27	0.60
1:H:7108:MSE:HB3	1:H:7109:PRO:HD3	1.82	0.60
1:H:7374:PRO:HG3	1:H:7380:ALA:HA	1.83	0.60
1:A:101:GLN:HB2	1:A:520:GLN:HE22	1.66	0.60
1:B:1223:GLN:HG2	1:B:1224:LYS:N	2.16	0.60
1:B:1310:LEU:HD23	1:B:1427:GLU:HG3	1.84	0.60
1:C:2546:PRO:HG2	1:C:2549:LYS:HD2	1.83	0.60
1:D:3315:ALA:HB3	1:D:3392:VAL:HG11	1.83	0.60
1:D:3389:ILE:CG2	1:D:3416:ILE:HG22	2.32	0.60
1:E:4338:GLN:HE21	1:E:4364:PRO:HB3	1.64	0.60
1:E:4452:VAL:O	1:E:4459:VAL:HA	2.01	0.60
1:F:5448:PRO:HB3	1:F:5464:GLN:OE1	2.00	0.60
1:G:6154:HIS:CE1	1:G:6156:LYS:HE2	2.35	0.60
1:G:6314:GLU:N	1:G:6317:LEU:CD1	2.65	0.60
1:H:7412:GLU:HA	1:H:7440:ARG:HH11	1.65	0.60
1:A:308:LEU:O	1:A:389:ILE:HD12	2.02	0.60
1:A:323:ILE:HG21	1:A:341:ILE:HD11	1.82	0.60
1:C:2351:VAL:HG22	1:C:2367:HIS:O	2.02	0.60
1:D:3166:ILE:HG22	1:D:3166:ILE:O	2.01	0.60
1:F:5456:ASP:OD1	1:F:5456:ASP:N	2.33	0.60
1:G:6491:PHE:O	1:G:6492:LEU:C	2.40	0.60
1:H:7159:VAL:HG23	1:H:7184:LEU:HD11	1.82	0.60
1:H:7468:VAL:O	1:H:7468:VAL:HG22	2.01	0.60
1:A:392:VAL:CG2	1:A:419:LEU:HD23	2.29	0.60
1:E:4359:ASP:OD2	1:E:4362:GLN:N	2.34	0.60
1:E:4370:PRO:HD2	1:E:4373:ILE:CD1	2.31	0.60
1:E:4453:LYS:CE	1:E:4457:GLY:HA2	2.32	0.60
1:F:5412:GLU:O	1:F:5440:ARG:HD2	2.01	0.60
1:G:6351:VAL:O	1:G:6366:THR:HG22	2.01	0.60
1:H:7389:ILE:HD12	1:H:7390:ILE:N	2.17	0.60
1:H:7416:ILE:HG12	1:H:7416:ILE:O	2.01	0.60
1:H:7531:THR:OG1	1:H:7532:GLU:N	2.35	0.60
1:H:7535:TYR:O	1:H:7538:LYS:N	2.32	0.60
1:A:89:GLN:O	1:A:91:ARG:N	2.34	0.60
1:B:1261:ASN:HD22	1:B:1261:ASN:N	1.96	0.60
1:C:2399:PHE:HB2	1:C:2427:GLU:O	2.01	0.60
1:D:3215:ASP:OD1	1:D:3216:PRO:HD2	2.02	0.60
1:D:3243:THR:HA	1:D:3247:GLY:O	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3453:LYS:HG2	1:D:3459:VAL:HG13	1.84	0.60
1:D:3505:GLU:N	1:D:3505:GLU:OE2	2.29	0.60
1:E:4123:TYR:CD2	1:E:4219:MSE:HE1	2.37	0.60
1:E:4432:GLU:O	1:E:4436:LEU:HB2	2.02	0.60
1:G:6243:THR:HA	1:G:6247:GLY:O	2.00	0.60
1:H:7158:VAL:HG22	1:H:7199:LEU:HD23	1.82	0.60
1:A:259:ASN:H	1:A:259:ASN:ND2	2.00	0.60
1:B:1116:VAL:HG13	1:B:1117:GLY:H	1.67	0.60
1:B:1420:SER:HB3	1:B:1425:GLN:HB3	1.82	0.60
1:D:3122:GLN:HA	1:D:3122:GLN:HE21	1.66	0.60
1:D:3276:PHE:HB3	1:D:3486:ILE:HD12	1.83	0.60
1:D:3352:LYS:N	1:D:3367:HIS:O	2.33	0.60
1:E:4067:ARG:HB2	1:F:5217:PHE:CE1	2.37	0.60
1:E:4120:CYS:SG	1:E:4179:ILE:HG12	2.41	0.60
1:G:6075:MSE:HG2	1:G:6080:GLU:HG2	1.82	0.60
1:H:7302:ILE:O	1:H:7304:GLU:N	2.35	0.60
1:H:7493:GLU:HA	1:H:7496:LYS:CD	2.31	0.60
1:B:1103:ASP:CG	1:B:1106:SER:HG	2.05	0.60
1:B:1164:GLU:HG3	1:B:1225:ARG:CZ	2.32	0.60
1:C:2238:PHE:CE1	1:C:2242:ILE:HG13	2.37	0.60
1:F:5068:PHE:CZ	1:F:5085:ILE:HD12	2.37	0.60
1:F:5176:GLY:C	1:F:5178:GLY:H	2.06	0.60
1:F:5310:LEU:O	1:F:5344:PHE:O	2.20	0.60
1:F:5376:THR:HG21	1:F:5378:GLU:OE2	2.02	0.60
1:G:6108:MSE:N	1:G:6109:PRO:HD2	2.17	0.60
1:H:7144:ARG:HH12	1:H:7244:ASP:HB3	1.66	0.60
1:A:273:TYR:HB3	4:A:8050:HOH:O	2.02	0.59
1:A:277:ASN:O	1:A:281:GLN:HB2	2.02	0.59
1:A:26:LYS:O	1:A:29:MSE:N	2.34	0.59
1:A:376:THR:CG2	1:A:378:GLU:H	2.14	0.59
1:B:1483:THR:HG21	1:B:1534:LEU:HD22	1.84	0.59
1:C:2182:GLY:O	1:C:2185:CYS:HB2	2.02	0.59
1:C:2338:GLN:HA	1:C:2341:ILE:HG13	1.84	0.59
1:C:2317:LEU:HD23	1:C:2361:TYR:HB3	1.85	0.59
1:F:5411:ASN:HD22	1:F:5414:PRO:HB3	1.66	0.59
1:H:7286:VAL:HG13	1:H:7470:ILE:CD1	2.32	0.59
1:H:7310:LEU:O	1:H:7344:PHE:O	2.21	0.59
1:A:416:ILE:HD13	1:A:416:ILE:H	1.67	0.59
1:A:535:TYR:OH	1:A:546:PRO:HD2	2.02	0.59
1:A:86:MSE:O	1:A:89:GLN:HB3	2.01	0.59
1:C:2303:SER:C	1:C:2340:LYS:HZ3	2.05	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2377:PHE:CZ	1:C:2389:ILE:HD11	2.37	0.59
1:D:3162:ASP:N	1:D:3162:ASP:OD1	2.35	0.59
1:D:3295:GLN:NE2	1:D:3305:HIS:HE1	1.99	0.59
1:D:3521:GLU:HA	1:D:3524:ILE:HD12	1.84	0.59
1:E:4235:ILE:O	1:E:4239:MSE:HG2	2.03	0.59
1:E:4384:LEU:O	1:E:4385:LYS:HE2	2.02	0.59
1:E:4511:ARG:HB2	1:E:4511:ARG:HH11	1.65	0.59
1:G:6103:ASP:O	1:G:6107:LEU:HD23	2.01	0.59
1:G:6352:LYS:HG3	1:G:6368:SER:CA	2.30	0.59
1:H:7060:THR:H	1:H:7063:ILE:CD1	2.15	0.59
1:H:7266:LEU:HD12	1:H:7266:LEU:O	2.02	0.59
1:A:71:ASN:HD22	1:A:71:ASN:N	1.98	0.59
1:D:3402:ASP:HA	1:D:3405:ARG:HG2	1.84	0.59
1:E:4300:LYS:HZ3	1:E:4305:HIS:HA	1.66	0.59
1:G:6161:THR:HA	1:G:6257:PHE:CE1	2.37	0.59
1:G:6184:LEU:O	1:G:6187:TYR:HB2	2.01	0.59
1:H:7416:ILE:HD12	1:H:7441:CYS:HB2	1.85	0.59
1:C:2261:ASN:ND2	1:C:2261:ASN:N	2.49	0.59
1:E:4212:LEU:O	1:E:4214:LYS:N	2.35	0.59
1:E:4437:THR:C	1:E:4439:GLY:N	2.56	0.59
1:E:4475:ALA:O	1:E:4479:ILE:HG12	2.02	0.59
1:F:5238:PHE:HE1	1:F:5242:ILE:HD11	1.67	0.59
1:A:269:TYR:HB3	1:A:273:TYR:HD1	1.66	0.59
1:A:477:ALA:CB	1:A:531:THR:HG22	2.32	0.59
1:B:1135:ILE:CG2	1:B:1143:VAL:HG22	2.32	0.59
1:B:1320:ALA:HA	1:B:1323:ILE:HD12	1.84	0.59
1:C:2210:ILE:CA	1:C:2213:LEU:HD12	2.32	0.59
1:C:2469:TYR:OH	1:C:2516:LEU:HD13	2.01	0.59
1:D:3207:THR:O	1:D:3224:LYS:HA	2.03	0.59
1:D:3376:THR:HG21	1:D:3378:GLU:HG2	1.83	0.59
1:F:5061:GLN:HA	1:F:5064:GLN:HG3	1.83	0.59
1:G:6062:ASP:OD1	1:G:6098:ARG:NH2	2.33	0.59
1:G:6498:LEU:O	1:G:6501:GLN:HB2	2.02	0.59
1:H:7026:LYS:N	1:H:7027:PRO:CD	2.65	0.59
1:H:7345:ASP:CG	1:H:7347:TYR:H	2.06	0.59
1:B:1240:LYS:HA	1:B:1243:THR:OG1	2.02	0.59
1:C:2210:ILE:HG22	1:C:2214:LYS:CD	2.32	0.59
1:D:3333:SER:HB3	1:D:3336:GLU:OE1	2.02	0.59
1:E:4116:VAL:HG13	1:E:4117:GLY:N	2.18	0.59
1:E:4239:MSE:HE3	1:E:4273:TYR:CD1	2.38	0.59
1:F:5283:THR:O	1:F:5286:VAL:HG23	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:6045:ARG:NH1	1:G:6058:ILE:HD13	2.17	0.59
1:G:6112:TYR:OH	1:G:6183:LYS:HE2	2.01	0.59
1:G:6352:LYS:HG2	1:G:6367:HIS:C	2.22	0.59
1:A:419:LEU:H	1:A:419:LEU:CD2	2.10	0.59
1:A:458:ARG:HB3	1:A:460:PHE:CE1	2.37	0.59
1:B:1401:PRO:CA	1:B:1404:ILE:HD12	2.32	0.59
1:C:2253:GLN:HG3	1:C:2276:PHE:CE2	2.38	0.59
1:C:2300:LYS:HG2	1:C:2304:GLU:CD	2.23	0.59
1:C:2416:ILE:HD13	1:C:2416:ILE:N	2.15	0.59
1:F:5253:GLN:HG3	1:F:5276:PHE:CE2	2.38	0.59
1:F:5454:LEU:HD12	1:F:5454:LEU:H	1.66	0.59
1:G:6174:VAL:HG21	1:G:6219:MSE:C	2.23	0.59
1:G:6276:PHE:C	1:G:6276:PHE:CD1	2.76	0.59
1:B:1046:GLN:HG3	1:B:1051:GLN:HG3	1.85	0.59
1:B:1300:LYS:NZ	1:B:1305:HIS:HA	2.18	0.59
1:B:1343:MSE:O	1:B:1350:LEU:HB2	2.03	0.59
1:B:1491:PHE:O	1:B:1494:ALA:HB3	2.02	0.59
1:C:2354:ARG:HE	1:C:2356:ALA:HB3	1.67	0.59
1:C:2422:PRO:C	1:C:2424:ALA:N	2.56	0.59
1:D:3165:ARG:HA	1:D:3170:GLY:HA2	1.84	0.59
1:D:3240:LYS:O	1:D:3244:ASP:HB2	2.03	0.59
1:D:3342:TRP:CZ3	1:D:3351:VAL:HG23	2.32	0.59
1:F:5332:LEU:HD23	1:F:5336:GLU:HB2	1.84	0.59
1:G:6310:LEU:HD21	1:G:6398:LEU:HB3	1.85	0.59
1:H:7207:THR:HG22	1:H:7213:LEU:HD21	1.83	0.59
1:H:7298:ILE:HD11	1:H:7442:LEU:HD21	1.85	0.59
1:A:309:PHE:CE1	1:A:390:ILE:HG13	2.38	0.59
1:A:388:THR:HG23	1:A:415:VAL:HB	1.83	0.59
1:B:1144:ARG:HH11	1:B:1244:ASP:HB3	1.67	0.59
1:C:2132:GLY:HA3	1:C:2177:MSE:CE	2.33	0.59
1:D:3184:LEU:O	1:D:3187:TYR:HB2	2.02	0.59
1:E:4301:PRO:HD2	1:E:4304:GLU:OE1	2.03	0.59
1:A:308:LEU:HD12	1:A:309:PHE:N	2.17	0.59
1:B:1440:ARG:HB3	1:B:1440:ARG:HH11	1.68	0.59
1:E:4266:LEU:O	1:E:4270:ARG:CB	2.50	0.59
1:E:4332:LEU:HD11	1:E:4340:LYS:HZ1	1.67	0.59
1:G:6079:LEU:HD13	1:G:6118:LEU:CD2	2.29	0.59
1:G:6260:HIS:CE1	1:G:6264:ARG:HE	2.20	0.59
1:G:6402:ASP:HA	1:G:6405:ARG:HG2	1.85	0.59
1:G:6478:VAL:HG12	1:G:6479:ILE:N	2.17	0.59
1:A:451:PRO:CA	1:A:460:PHE:O	2.49	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2238:PHE:CE1	1:C:2242:ILE:CG1	2.86	0.58
1:C:2261:ASN:HB3	1:C:2265:PHE:CE1	2.38	0.58
1:C:2499:THR:O	1:C:2501:GLN:N	2.34	0.58
1:D:3343:MSE:O	1:D:3350:LEU:HB2	2.02	0.58
1:D:3359:ASP:OD2	1:D:3362:GLN:N	2.36	0.58
1:F:5512:LEU:H	1:F:5512:LEU:HD12	1.67	0.58
1:G:6196:ASP:OD1	1:G:6196:ASP:N	2.34	0.58
1:C:2106:SER:O	1:C:2109:PRO:HD2	2.03	0.58
1:E:4416:ILE:HG12	1:E:4443:PHE:CD1	2.37	0.58
1:F:5239:MSE:HE2	1:F:5273:TYR:CD1	2.37	0.58
1:F:5431:GLU:C	1:F:5433:ALA:H	2.04	0.58
1:A:243:THR:CG2	1:A:248:ARG:HA	2.31	0.58
1:A:303:SER:HA	1:A:340:LYS:NZ	2.18	0.58
1:B:1419:LEU:N	1:B:1419:LEU:HD22	2.17	0.58
1:C:2313:GLY:O	1:C:2315:ALA:N	2.36	0.58
1:D:3166:ILE:CG2	1:D:3172:LEU:HD12	2.33	0.58
1:F:5238:PHE:CE1	1:F:5242:ILE:HD11	2.39	0.58
1:H:7104:ILE:HG13	1:H:7108:MSE:CE	2.33	0.58
1:H:7177:MSE:O	1:H:7181:VAL:HG23	2.04	0.58
1:H:7093:GLU:OE1	1:H:7195:PRO:HB2	2.02	0.58
1:H:7194:ARG:HG3	1:H:7197:ARG:NH1	2.17	0.58
1:H:7209:ASN:O	1:H:7212:LEU:HB2	2.04	0.58
1:H:7531:THR:O	1:H:7532:GLU:C	2.42	0.58
1:H:7533:TYR:CD2	1:H:7533:TYR:C	2.76	0.58
1:B:1402:ASP:O	1:B:1405:ARG:HG2	2.03	0.58
1:E:4456:ASP:OD1	1:E:4458:ARG:HB2	2.04	0.58
1:F:5261:ASN:HB3	1:F:5265:PHE:CE1	2.38	0.58
1:F:5352:LYS:N	1:F:5367:HIS:O	2.34	0.58
1:G:6536:ALA:HA	1:G:6538:LYS:NZ	2.18	0.58
1:A:412:GLU:O	1:A:413:ARG:HG2	2.03	0.58
1:B:1370:PRO:HD2	1:B:1373:ILE:HD11	1.85	0.58
1:B:1416:ILE:O	1:B:1416:ILE:HG12	2.01	0.58
1:C:2352:LYS:HG3	1:C:2368:SER:HA	1.85	0.58
1:C:2376:THR:HB	1:C:2379:ASP:H	1.68	0.58
1:D:3280:ILE:CD1	4:D:8022:HOH:O	2.51	0.58
1:E:4505:GLU:H	1:E:4505:GLU:CD	2.06	0.58
1:E:4559:ARG:HB3	1:E:4561:GLU:HG2	1.86	0.58
1:G:6086:MSE:CE	1:G:6086:MSE:CA	2.79	0.58
1:H:7280:ILE:HG22	1:H:7281:GLN:N	2.19	0.58
1:H:7566:LEU:HD22	1:H:7567:PRO:HD2	1.84	0.58
1:A:194:ARG:O	1:A:197:ARG:HB2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:402:ASP:HA	1:A:405:ARG:CD	2.29	0.58
1:A:481:CYS:SG	1:A:531:THR:HB	2.44	0.58
1:B:1133:LEU:HD13	1:B:1150:TRP:CE3	2.39	0.58
1:C:2387:SER:O	1:C:2415:VAL:HG23	2.03	0.58
1:C:2453:LYS:HE3	1:C:2457:GLY:HA2	1.83	0.58
1:E:4421:ASN:HB3	1:E:4422:PRO:HA	1.85	0.58
1:G:6122:GLN:O	1:G:6125:HIS:HB2	2.04	0.58
1:G:6279:ASP:OD1	1:G:6279:ASP:N	2.37	0.58
1:A:270:ARG:HG2	1:A:271:GLU:HG2	1.86	0.58
1:B:1041:THR:HG23	1:B:1044:GLU:CG	2.34	0.58
1:B:1346:LYS:HD2	1:B:1347:TYR:CE2	2.39	0.58
1:B:1483:THR:OG1	1:B:1534:LEU:HD13	2.04	0.58
1:C:2137:ILE:HA	1:C:2234:LEU:CD2	2.34	0.58
1:G:6038:MSE:O	1:G:6045:ARG:NH2	2.37	0.58
1:H:7359:ASP:OD2	1:H:7362:GLN:N	2.37	0.58
1:C:2342:TRP:HZ3	1:C:2351:VAL:HG23	1.69	0.58
1:C:2523:SER:HA	1:C:2526:ILE:HD12	1.86	0.58
1:D:3082:TYR:O	1:D:3085:ILE:HG22	2.04	0.58
1:D:3404:ILE:HD12	1:D:3436:LEU:HD22	1.84	0.58
1:D:3094:LYS:HB3	1:D:3562:TYR:CE2	2.39	0.58
1:E:4293:ALA:HB3	1:E:4512:LEU:HB3	1.85	0.58
1:E:4317:LEU:N	1:E:4317:LEU:HD12	2.19	0.58
1:F:5065:ALA:O	1:F:5068:PHE:HB3	2.03	0.58
1:G:6307:ILE:HG22	1:G:6308:LEU:N	2.18	0.58
1:G:6314:GLU:N	1:G:6317:LEU:HD13	2.19	0.58
1:A:176:GLY:C	1:A:178:GLY:H	2.06	0.58
1:A:288:LEU:HD22	1:A:322:LEU:HD23	1.86	0.58
1:A:309:PHE:HD2	1:A:343:MSE:HG3	1.68	0.58
1:B:1137:ILE:HG22	1:B:1221:LEU:HD23	1.86	0.58
1:B:1458:ARG:HB3	1:B:1460:PHE:CZ	2.39	0.58
1:B:1525:ASN:HA	1:B:1528:ILE:HG13	1.84	0.58
1:C:2044:GLU:O	1:C:2048:LEU:HD23	2.03	0.58
1:C:2270:ARG:HG3	1:C:2271:GLU:H	1.69	0.58
1:C:2537:ASN:HD22	1:C:2537:ASN:N	2.02	0.58
1:D:3543:TYR:C	1:D:3543:TYR:CD2	2.77	0.58
1:E:4315:ALA:CB	1:E:4392:VAL:HG11	2.33	0.58
1:E:4397:ARG:HA	1:E:4427:GLU:O	2.03	0.58
1:E:4526:ILE:O	1:E:4530:VAL:HG23	2.04	0.58
1:F:5085:ILE:HG23	1:F:5086:MSE:HE2	1.85	0.58
1:G:6300:LYS:O	1:G:6302:ILE:N	2.36	0.58
1:G:6352:LYS:HG2	1:G:6367:HIS:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:7046:GLN:HG3	1:H:7051:GLN:HG3	1.86	0.58
1:A:253:GLN:HG3	1:A:276:PHE:CE2	2.39	0.58
1:B:1093:GLU:O	1:B:1094:LYS:C	2.41	0.58
1:C:2327:MSE:HE1	1:C:2337:ALA:O	2.03	0.58
1:C:2383:ILE:O	1:C:2385:LYS:NZ	2.35	0.58
1:E:4155:VAL:HB	1:E:4246:TYR:CD2	2.39	0.58
1:E:4374:PRO:CB	1:E:4383:ILE:HD12	2.34	0.58
1:E:4400:THR:O	1:E:4403:VAL:HB	2.04	0.58
1:F:5494:ALA:O	1:F:5497:ALA:HB3	2.04	0.58
1:H:7300:LYS:O	1:H:7302:ILE:N	2.36	0.58
1:A:175:TYR:OH	1:A:218:TYR:HA	2.04	0.57
1:A:298:ILE:HD11	1:A:442:LEU:CD1	2.31	0.57
1:A:315:ALA:O	1:A:319:ILE:HD12	2.04	0.57
1:A:466:ASN:CB	1:A:468:VAL:HG12	2.31	0.57
1:A:528:ILE:O	1:A:532:GLU:HG3	2.04	0.57
1:D:3351:VAL:HG21	1:D:3370:PRO:HD3	1.85	0.57
1:E:4133:LEU:HD12	1:F:5052:GLY:O	2.04	0.57
1:E:4289:ALA:HA	1:E:4499:THR:OG1	2.04	0.57
1:G:6350:LEU:HD22	1:G:6354:ARG:NH1	2.19	0.57
1:G:6354:ARG:HG3	1:G:6356:ALA:H	1.68	0.57
1:G:6289:ALA:O	1:G:6499:THR:OG1	2.21	0.57
1:G:6537:ASN:O	1:G:6539:MSE:HG3	2.04	0.57
1:H:7086:MSE:CE	1:H:7086:MSE:HA	2.33	0.57
1:H:7303:SER:O	1:H:7340:LYS:HE3	2.03	0.57
1:H:7354:ARG:HG2	1:H:7358:ILE:HD11	1.86	0.57
1:A:417:PHE:CE2	1:A:444:ALA:HB3	2.39	0.57
1:A:424:ALA:HB3	1:A:425:GLN:HE21	1.68	0.57
1:C:2227:ARG:NH1	1:C:2227:ARG:CG	2.61	0.57
1:C:2411:ASN:HD22	1:C:2414:PRO:HB3	1.69	0.57
1:D:3077:SER:OG	1:D:3080:GLU:HB2	2.04	0.57
1:D:3106:SER:C	1:D:3109:PRO:HD2	2.24	0.57
1:D:3335:GLN:O	1:D:3339:LYS:HB2	2.03	0.57
1:E:4163:GLY:O	1:E:4171:ASP:HA	2.04	0.57
1:G:6060:THR:H	1:G:6063:ILE:HD12	1.69	0.57
1:A:397:ARG:N	1:A:397:ARG:HD2	2.19	0.57
1:B:1041:THR:HG23	1:B:1044:GLU:CD	2.25	0.57
1:D:3553:VAL:O	1:D:3555:GLU:N	2.37	0.57
1:E:4309:PHE:HB2	1:E:4343:MSE:HG2	1.86	0.57
1:F:5176:GLY:C	1:F:5178:GLY:N	2.54	0.57
1:G:6205:VAL:HG21	1:G:6231:TYR:HE1	1.69	0.57
1:A:144:ARG:HH12	1:A:244:ASP:HB3	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:ARG:CZ	1:A:259:ASN:HD21	2.16	0.57
1:A:187:TYR:O	1:A:193:ILE:HD12	2.04	0.57
1:A:31:ASN:OD1	1:A:33:ARG:N	2.38	0.57
1:A:422:PRO:HD2	1:A:425:GLN:HG2	1.85	0.57
1:A:572:TRP:NE1	1:D:3138:SER:O	2.38	0.57
1:C:2257:PHE:CB	1:C:2262:ALA:HB2	2.34	0.57
1:D:3258:GLY:O	1:D:3259:ASN:C	2.42	0.57
1:E:4502:LEU:HD12	1:E:4507:LEU:HD22	1.86	0.57
1:E:4535:TYR:CD2	1:E:4540:ALA:HB3	2.39	0.57
1:F:5320:ALA:HB1	1:F:5365:PHE:CZ	2.40	0.57
1:A:324:VAL:O	1:A:327:MSE:N	2.34	0.57
1:C:2416:ILE:HG12	1:C:2443:PHE:HD1	1.67	0.57
1:D:3381:VAL:HG13	1:D:3407:MSE:HE1	1.85	0.57
1:E:4295:GLN:HE22	1:E:4305:HIS:CE1	2.23	0.57
1:E:4350:LEU:HD13	1:E:4354:ARG:HD3	1.87	0.57
1:F:5166:ILE:HG23	1:F:5179:ILE:HD11	1.86	0.57
1:G:6030:LEU:HD12	1:H:7030:LEU:HB3	1.85	0.57
1:G:6086:MSE:HE1	1:G:6111:VAL:HG22	1.87	0.57
1:G:6095:LEU:HG	1:G:6099:ILE:CD1	2.33	0.57
1:G:6247:GLY:O	1:G:6250:THR:HB	2.04	0.57
1:H:7159:VAL:HA	1:H:7253:GLN:O	2.05	0.57
1:H:7511:ARG:HH11	1:H:7511:ARG:HB2	1.68	0.57
1:A:416:ILE:CD1	1:A:441:CYS:HB2	2.34	0.57
1:B:1122:GLN:HE21	1:B:1122:GLN:HA	1.68	0.57
1:C:2123:TYR:HD2	1:C:2219:MSE:CE	2.16	0.57
1:C:2300:LYS:HE2	1:C:2304:GLU:HB2	1.86	0.57
1:C:2323:ILE:HG22	1:C:2327:MSE:HE2	1.86	0.57
1:C:2351:VAL:HG13	1:C:2352:LYS:N	2.18	0.57
1:D:3372:SER:HB2	1:D:3383:ILE:CD1	2.34	0.57
1:E:4179:ILE:HB	1:E:4180:PRO:HD3	1.85	0.57
1:E:4333:SER:H	1:E:4336:GLU:CD	2.07	0.57
1:G:6204:ASP:OD2	1:G:6221:LEU:N	2.36	0.57
1:G:6249:ASN:OD1	1:G:6249:ASN:C	2.42	0.57
1:H:7123:TYR:HB3	1:H:7175:TYR:CD2	2.38	0.57
1:C:2044:GLU:HA	1:C:2048:LEU:HD23	1.85	0.57
1:C:2130:PRO:C	1:C:2131:LYS:HG2	2.25	0.57
1:C:2144:ARG:NH1	1:C:2244:ASP:HB3	2.20	0.57
1:D:3400:THR:HG23	1:D:3403:VAL:HG23	1.87	0.57
1:F:5210:ILE:HG22	1:F:5214:LYS:HE2	1.86	0.57
1:G:6281:GLN:HG2	1:G:6491:PHE:CE1	2.38	0.57
1:G:6467:ASN:C	1:G:6469:TYR:N	2.58	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:7497:ALA:O	1:H:7501:GLN:HG2	2.04	0.57
1:H:7292:LEU:HB3	1:H:7499:THR:HG21	1.86	0.57
1:A:26:LYS:N	1:A:27:PRO:CD	2.68	0.57
1:B:1505:GLU:OE2	1:B:1505:GLU:N	2.38	0.57
1:C:2286:VAL:HG11	1:C:2466:ASN:O	2.05	0.57
1:C:2402:ASP:HA	1:C:2405:ARG:HG2	1.87	0.57
1:D:3137:ILE:C	1:D:3139:ASP:H	2.08	0.57
1:D:3437:THR:O	1:D:3438:GLU:HB2	2.05	0.57
1:E:4357:LYS:N	1:E:4357:LYS:HZ2	2.03	0.57
1:E:4549:LYS:O	1:E:4553:VAL:HG23	2.05	0.57
1:G:6466:ASN:CB	1:G:6468:VAL:HG12	2.35	0.57
1:H:7168:GLY:C	1:H:7169:LEU:HD12	2.26	0.57
1:H:7266:LEU:HD21	1:H:7281:GLN:NE2	2.19	0.57
1:C:2036:LYS:HG2	1:C:2562:TYR:CE2	2.39	0.57
1:D:3135:ILE:HD11	1:D:3143:VAL:HG13	1.87	0.57
1:D:3266:LEU:O	1:D:3266:LEU:HD12	2.05	0.57
1:F:5271:GLU:HA	1:F:5271:GLU:OE1	2.04	0.57
1:G:6166:ILE:HD13	1:G:6256:ASP:CB	2.34	0.57
1:G:6162:ASP:O	1:G:6225:ARG:NH2	2.37	0.57
1:A:86:MSE:HE2	1:A:86:MSE:CA	2.35	0.57
1:D:3255:GLU:OE1	1:D:3256:ASP:N	2.35	0.57
1:F:5308:LEU:HA	1:F:5342:TRP:O	2.05	0.57
1:F:5454:LEU:HD12	1:F:5458:ARG:O	2.04	0.57
1:G:6312:ALA:CB	1:G:6343:MSE:HE3	2.34	0.57
1:H:7255:GLU:O	1:H:7257:PHE:N	2.38	0.57
1:A:540:ALA:C	1:A:541:PHE:HD2	2.08	0.56
1:C:2414:PRO:HD2	1:C:2441:CYS:HA	1.86	0.56
1:D:3163:GLY:O	1:D:3171:ASP:HA	2.05	0.56
1:D:3199:LEU:HD12	1:D:3200:PRO:N	2.19	0.56
1:D:3396:GLY:O	1:D:3427:GLU:HA	2.05	0.56
1:E:4126:ILE:O	1:E:4128:ARG:HD2	2.05	0.56
1:F:5419:LEU:N	1:F:5419:LEU:HD22	2.18	0.56
1:F:5435:THR:OG1	1:F:5436:LEU:HD12	2.05	0.56
1:F:5470:ILE:HD11	1:F:5498:LEU:HD22	1.86	0.56
1:F:5559:ARG:HH11	1:F:5559:ARG:CG	2.18	0.56
1:F:5566:LEU:CD2	1:F:5567:PRO:HD2	2.34	0.56
1:G:6177:MSE:CE	1:G:6180:PRO:HB2	2.35	0.56
1:H:7259:ASN:O	1:H:7260:HIS:C	2.43	0.56
1:A:176:GLY:C	1:A:178:GLY:N	2.59	0.56
1:A:412:GLU:C	1:A:440:ARG:HH11	2.08	0.56
1:B:1152:GLU:O	1:B:1246:TYR:OH	2.17	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1253:GLN:HE22	1:B:1255:GLU:CG	2.18	0.56
1:B:1391:GLY:CA	1:B:1427:GLU:HG2	2.36	0.56
1:C:2099:ILE:HA	1:C:2102:ASP:HB2	1.88	0.56
1:D:3100:LEU:C	1:D:3102:ASP:H	2.09	0.56
1:D:3122:GLN:O	1:D:3125:HIS:HB2	2.05	0.56
1:D:3443:PHE:O	1:D:3512:LEU:HD13	2.05	0.56
1:E:4376:THR:O	1:E:4379:ASP:HB2	2.04	0.56
1:E:4502:LEU:HD21	1:E:4513:TYR:N	2.20	0.56
1:F:5060:THR:OG1	1:F:5063:ILE:HD12	2.05	0.56
1:F:5144:ARG:NH1	1:F:5244:ASP:HB3	2.20	0.56
1:F:5349:LEU:HD21	1:F:5351:VAL:HG23	1.87	0.56
1:G:6491:PHE:O	1:G:6494:ALA:N	2.38	0.56
1:H:7554:LYS:HB3	4:H:8039:HOH:O	2.04	0.56
1:B:1161:THR:HA	1:B:1257:PHE:CE1	2.40	0.56
1:B:1397:ARG:HD3	1:B:1428:CYS:HA	1.86	0.56
1:B:1504:ASP:HA	1:B:1507:LEU:HB2	1.87	0.56
1:C:2101:GLN:HA	1:C:2104:ILE:HB	1.86	0.56
1:D:3094:LYS:HB3	1:D:3562:TYR:HE2	1.69	0.56
1:E:4228:THR:OG1	1:E:4229:GLN:N	2.37	0.56
1:E:4474:VAL:HG12	1:E:4475:ALA:N	2.21	0.56
1:G:6207:THR:HG23	1:G:6213:LEU:CD2	2.34	0.56
1:G:6302:ILE:HG22	1:G:6340:LYS:HZ1	1.68	0.56
1:G:6474:VAL:O	1:G:6475:ALA:C	2.42	0.56
1:H:7319:ILE:O	1:H:7323:ILE:HG13	2.05	0.56
1:A:294:ALA:O	1:A:297:VAL:HG13	2.06	0.56
1:A:78:PRO:HA	1:A:81:LYS:HG3	1.87	0.56
1:B:1374:PRO:HB3	1:B:1383:ILE:HD12	1.87	0.56
1:B:1388:THR:CG2	1:B:1415:VAL:HB	2.29	0.56
1:C:2540:ALA:C	1:C:2541:PHE:HD2	2.09	0.56
1:D:3079:LEU:HD11	1:D:3119:ALA:HA	1.87	0.56
1:D:3133:LEU:HD23	1:D:3199:LEU:HD21	1.88	0.56
1:E:4155:VAL:HB	1:E:4246:TYR:CG	2.39	0.56
1:F:5157:ALA:O	1:F:5198:CYS:HA	2.05	0.56
1:F:5283:THR:HG22	1:F:5284:ALA:N	2.20	0.56
1:G:6320:ALA:O	1:G:6324:VAL:HG23	2.04	0.56
1:G:6524:ILE:O	1:G:6527:ALA:HB3	2.04	0.56
1:A:143:VAL:O	1:A:147:VAL:HG23	2.05	0.56
1:A:44:GLU:HG3	1:A:566:LEU:HG	1.86	0.56
1:C:2234:LEU:O	1:C:2234:LEU:HD12	2.04	0.56
1:A:572:TRP:NE1	1:D:3139:ASP:OD1	2.37	0.56
1:D:3308:LEU:HB3	1:D:3389:ILE:CD1	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3332:LEU:HD22	1:D:3337:ALA:HB2	1.88	0.56
1:E:4174:VAL:CG1	1:E:4220:GLY:HA3	2.36	0.56
1:E:4352:LYS:HG3	1:E:4368:SER:N	2.20	0.56
1:H:7108:MSE:HB3	1:H:7109:PRO:CD	2.35	0.56
1:H:7305:HIS:O	1:H:7340:LYS:HG2	2.05	0.56
1:A:179:ILE:HB	1:A:180:PRO:HD3	1.88	0.56
1:A:300:LYS:HD2	1:A:304:GLU:CD	2.26	0.56
1:A:91:ARG:HG3	1:B:1129:ARG:NH2	2.20	0.56
1:B:1143:VAL:O	1:B:1147:VAL:HG23	2.04	0.56
1:C:2386:PRO:HB2	1:C:2388:THR:O	2.06	0.56
1:C:2429:THR:HG23	1:C:2432:GLU:CD	2.26	0.56
1:F:5363:GLU:HA	1:F:5366:THR:OG1	2.05	0.56
1:G:6314:GLU:CA	1:G:6317:LEU:HD13	2.36	0.56
1:G:6378:GLU:HA	1:G:6381:VAL:HB	1.87	0.56
1:G:6413:ARG:HB3	1:G:6442:LEU:HD11	1.87	0.56
1:B:1097:TYR:O	1:B:1100:LEU:HB3	2.06	0.56
1:B:1295:GLN:NE2	1:B:1305:HIS:NE2	2.54	0.56
1:B:1489:SER:HB2	1:B:1533:TYR:OH	2.06	0.56
1:C:2341:ILE:HB	1:C:2365:PHE:HD2	1.70	0.56
1:D:3266:LEU:C	1:D:3266:LEU:HD12	2.25	0.56
1:E:4108:MSE:HB3	1:E:4109:PRO:HD3	1.86	0.56
1:E:4300:LYS:NZ	1:E:4305:HIS:HA	2.20	0.56
1:F:5208:ASP:O	1:F:5210:ILE:HD13	2.05	0.56
1:F:5388:THR:HG23	1:F:5415:VAL:CB	2.27	0.56
1:G:6243:THR:CG2	1:G:6248:ARG:HA	2.35	0.56
1:H:7258:GLY:O	1:H:7260:HIS:N	2.39	0.56
1:H:7266:LEU:CD2	1:H:7277:ASN:H	2.19	0.56
1:H:7416:ILE:CD1	1:H:7441:CYS:HB2	2.36	0.56
1:H:7430:ALA:O	1:H:7433:ALA:HB3	2.05	0.56
1:A:187:TYR:O	1:A:191:ALA:HB3	2.05	0.56
1:B:1133:LEU:HB2	1:B:1199:LEU:HD11	1.87	0.56
1:B:1287:ALA:O	1:B:1290:GLY:N	2.37	0.56
1:B:1354:ARG:HE	1:B:1358:ILE:HD11	1.71	0.56
1:B:1451:PRO:HA	1:B:1460:PHE:O	2.05	0.56
1:B:1518:ASN:O	1:B:1522:VAL:HG23	2.04	0.56
1:D:3245:ARG:HD3	1:D:3246:TYR:CE1	2.39	0.56
1:D:3352:LYS:CB	1:D:3368:SER:HA	2.36	0.56
1:E:4328:VAL:HG12	1:E:4329:GLU:N	2.21	0.56
1:E:4381:VAL:O	1:E:4386:PRO:HD3	2.06	0.56
1:G:6526:ILE:O	1:G:6530:VAL:HG23	2.05	0.56
1:H:7082:TYR:C	1:H:7082:TYR:CD2	2.78	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:VAL:HB	1:A:237:GLU:HG2	1.87	0.56
1:A:407:MSE:HG3	1:A:414:PRO:HB3	1.87	0.56
1:B:1166:ILE:HG22	1:B:1166:ILE:O	2.05	0.56
1:B:1401:PRO:HB3	1:B:1436:LEU:HD21	1.87	0.56
1:B:1453:LYS:HA	1:B:1458:ARG:O	2.05	0.56
1:C:2123:TYR:HB3	1:C:2175:TYR:CD2	2.41	0.56
1:D:3412:GLU:HA	1:D:3440:ARG:NH1	2.20	0.56
1:D:3156:LYS:HD2	3:D:3602:NAD:O2B	2.06	0.56
1:G:6166:ILE:HG21	1:G:6172:LEU:HD12	1.87	0.56
1:G:6261:ASN:O	1:G:6264:ARG:HG2	2.06	0.56
1:G:6527:ALA:O	1:G:6531:THR:HG23	2.06	0.56
1:G:6549:LYS:O	1:G:6552:TYR:HB3	2.04	0.56
1:H:7302:ILE:O	1:H:7304:GLU:OE2	2.24	0.56
1:A:376:THR:HG22	1:A:378:GLU:H	1.68	0.56
1:C:2238:PHE:O	1:C:2242:ILE:HG12	2.06	0.56
1:D:3075:MSE:HG3	1:D:3080:GLU:OE1	2.05	0.56
1:D:3432:GLU:HG2	4:D:8007:HOH:O	2.06	0.56
1:E:4308:LEU:HB3	1:E:4389:ILE:HD11	1.87	0.56
1:G:6384:LEU:O	1:G:6385:LYS:HB2	2.06	0.56
1:H:7311:GLY:HA3	1:H:7392:VAL:O	2.06	0.56
1:H:7313:GLY:O	1:H:7314:GLU:C	2.44	0.56
1:B:1165:ARG:HD3	1:B:1258:GLY:HA2	1.88	0.56
1:B:1413:ARG:HA	1:B:1440:ARG:O	2.06	0.56
1:C:2569:VAL:O	1:C:2570:TYR:HB3	2.06	0.56
1:D:3047:MSE:C	1:D:3048:LEU:HD22	2.26	0.56
1:D:3150:TRP:HE1	1:D:3152:GLU:HB2	1.71	0.56
1:D:3298:ILE:HD11	1:D:3413:ARG:HB3	1.87	0.56
1:G:6205:VAL:HG11	1:G:6231:TYR:HD1	1.71	0.56
1:G:6370:PRO:HD2	1:G:6373:ILE:CD1	2.36	0.56
1:G:6490:VAL:O	1:G:6493:GLU:HB3	2.05	0.56
1:A:323:ILE:O	1:A:324:VAL:C	2.43	0.55
1:A:399:PHE:HA	1:A:403:VAL:HG11	1.86	0.55
1:A:451:PRO:HG3	1:A:461:THR:OG1	2.06	0.55
1:A:559:ARG:HG3	1:A:561:GLU:CG	2.31	0.55
1:B:1351:VAL:CG2	1:B:1369:ALA:HA	2.33	0.55
1:B:1351:VAL:HG11	1:B:1369:ALA:HB2	1.87	0.55
1:D:3372:SER:O	1:D:3374:PRO:HD3	2.06	0.55
1:E:4363:GLU:CB	1:E:4364:PRO:HD3	2.35	0.55
1:E:4541:PHE:HE1	1:H:7543:TYR:CE2	2.24	0.55
1:G:6234:LEU:O	1:G:6237:GLU:HB3	2.07	0.55
1:G:6253:GLN:NE2	1:G:6278:ASP:CB	2.68	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:6401:PRO:CA	1:G:6436:LEU:HD21	2.35	0.55
1:A:431:GLU:OE2	1:A:435:THR:HG21	2.07	0.55
1:A:475:ALA:O	1:A:479:ILE:HG12	2.06	0.55
1:B:1235:ILE:N	1:B:1235:ILE:HD13	2.21	0.55
1:B:1239:MSE:O	1:B:1243:THR:OG1	2.24	0.55
1:B:1239:MSE:HE1	1:B:1252:ILE:HD12	1.87	0.55
1:C:2177:MSE:HE1	1:C:2200:PRO:HG2	1.88	0.55
1:C:2177:MSE:O	1:C:2181:VAL:HG23	2.06	0.55
1:C:2153:ASN:O	1:C:2246:TYR:HE2	1.88	0.55
1:D:3416:ILE:O	1:D:3416:ILE:HG12	2.05	0.55
1:F:5286:VAL:HG21	1:F:5467:ASN:OD1	2.06	0.55
1:F:5302:ILE:HA	1:F:5305:HIS:CE1	2.41	0.55
1:F:5351:VAL:HG13	1:F:5352:LYS:N	2.21	0.55
1:F:5452:VAL:O	1:F:5459:VAL:HA	2.06	0.55
1:F:5487:SER:OG	1:F:5539:MSE:HE1	2.05	0.55
1:H:7518:ASN:O	1:H:7522:VAL:HG23	2.05	0.55
1:B:1425:GLN:NE2	1:B:1425:GLN:N	2.54	0.55
1:C:2026:LYS:N	1:C:2027:PRO:CD	2.70	0.55
1:C:2103:ASP:OD2	1:C:2106:SER:HB2	2.05	0.55
1:C:2559:ARG:HB3	1:C:2561:GLU:HG2	1.88	0.55
1:D:3210:ILE:O	1:D:3214:LYS:HD2	2.06	0.55
1:D:3309:PHE:CD1	1:D:3390:ILE:HB	2.42	0.55
1:D:3320:ALA:O	1:D:3324:VAL:HG23	2.07	0.55
1:D:3350:LEU:HD22	1:D:3354:ARG:HH12	1.70	0.55
1:D:3378:GLU:O	1:D:3381:VAL:HB	2.07	0.55
1:D:3521:GLU:N	1:D:3524:ILE:HD12	2.21	0.55
1:F:5033:ARG:NE	1:F:5093:GLU:OE1	2.39	0.55
1:F:5327:MSE:HE2	1:F:5341:ILE:HD11	1.87	0.55
1:F:5566:LEU:HD22	1:F:5567:PRO:HD2	1.87	0.55
1:G:6026:LYS:HD3	1:H:7151:PRO:HG3	1.87	0.55
1:G:6069:HIS:O	1:G:6073:LYS:HB2	2.06	0.55
1:G:6407:MSE:HA	1:G:6410:ILE:HD12	1.88	0.55
1:H:7397:ARG:HA	1:H:7427:GLU:C	2.27	0.55
1:H:7437:THR:HG21	1:H:7441:CYS:HB3	1.89	0.55
1:A:27:PRO:HA	1:A:30:LEU:HB2	1.87	0.55
1:A:454:LEU:HD13	1:A:458:ARG:HB2	1.88	0.55
1:B:1344:PHE:HD1	1:B:1349:LEU:HB2	1.72	0.55
1:B:1502:LEU:CD1	1:B:1506:GLU:HB3	2.35	0.55
1:C:2174:VAL:HG23	1:C:2219:MSE:HE3	1.88	0.55
1:C:2358:ILE:HG22	1:C:2362:GLN:CB	2.35	0.55
1:D:3116:VAL:HG21	1:D:3179:ILE:HD13	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3381:VAL:HG13	1:D:3407:MSE:CE	2.36	0.55
1:D:3543:TYR:HB2	1:D:3544:PRO:HA	1.87	0.55
1:F:5050:LEU:O	1:F:5053:LEU:HB2	2.07	0.55
1:F:5177:MSE:HE3	1:F:5181:VAL:HG23	1.88	0.55
1:G:6358:ILE:HA	1:G:6362:GLN:OE1	2.05	0.55
1:H:7317:LEU:H	1:H:7317:LEU:HD12	1.71	0.55
1:A:376:THR:HG22	1:A:379:ASP:H	1.71	0.55
1:B:1401:PRO:HA	1:B:1436:LEU:CD2	2.36	0.55
1:D:3376:THR:HG22	1:D:3378:GLU:H	1.72	0.55
1:E:4212:LEU:C	1:E:4214:LYS:H	2.10	0.55
1:E:4416:ILE:N	1:E:4416:ILE:HD13	2.21	0.55
1:F:5423:THR:CG2	1:F:5423:THR:O	2.54	0.55
1:G:6352:LYS:N	1:G:6367:HIS:O	2.39	0.55
1:H:7421:ASN:HB3	1:H:7422:PRO:HA	1.88	0.55
1:A:301:PRO:O	1:A:303:SER:N	2.40	0.55
1:C:2384:LEU:O	1:C:2385:LYS:HE2	2.07	0.55
1:C:2469:TYR:O	1:C:2470:ILE:HD13	2.07	0.55
1:D:3066:LEU:O	1:D:3067:ARG:C	2.44	0.55
1:H:7099:ILE:CA	1:H:7102:ASP:HB2	2.37	0.55
1:H:7255:GLU:OE2	1:H:7279:ASP:OD1	2.23	0.55
1:B:1535:TYR:CD1	1:B:1549:LYS:HE3	2.42	0.55
1:D:3264:ARG:HG3	1:D:3265:PHE:H	1.70	0.55
1:E:4301:PRO:O	1:E:4303:SER:N	2.39	0.55
1:E:4295:GLN:NE2	1:E:4305:HIS:HE1	2.05	0.55
1:E:4315:ALA:O	1:E:4319:ILE:HD12	2.06	0.55
1:E:4535:TYR:CD2	1:E:4540:ALA:CB	2.89	0.55
1:F:5036:LYS:HB3	1:F:5039:ALA:HB3	1.89	0.55
1:F:5058:ILE:HD13	1:F:5058:ILE:N	2.20	0.55
1:F:5071:ASN:O	1:F:5075:MSE:HE3	2.07	0.55
1:F:5431:GLU:C	1:F:5433:ALA:N	2.60	0.55
1:F:5564:SER:C	1:F:5565:LEU:HD23	2.27	0.55
1:G:6357:LYS:O	1:G:6358:ILE:HG13	2.07	0.55
1:G:6384:LEU:O	1:G:6385:LYS:HE3	2.07	0.55
1:G:6454:LEU:CD1	1:G:6458:ARG:HB3	2.29	0.55
1:H:7133:LEU:HD21	1:H:7146:ILE:HG22	1.89	0.55
1:H:7147:VAL:O	1:H:7245:ARG:NH1	2.37	0.55
1:A:172:LEU:O	1:A:175:TYR:HB2	2.07	0.55
1:A:210:ILE:HA	1:A:213:LEU:HB2	1.88	0.55
1:A:454:LEU:CD1	1:A:458:ARG:HB2	2.37	0.55
1:A:512:LEU:O	4:A:8037:HOH:O	2.18	0.55
1:B:1072:LEU:HD11	1:B:1081:LYS:HB3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1210:ILE:N	1:B:1210:ILE:HD13	2.21	0.55
1:B:1217:PHE:O	1:B:1218:TYR:C	2.45	0.55
1:D:3408:ALA:HA	1:D:3414:PRO:HG3	1.88	0.55
1:F:5293:ALA:O	1:F:5297:VAL:HG13	2.07	0.55
1:G:6024:LYS:CA	1:G:6028:LEU:HD22	2.33	0.55
1:G:6172:LEU:O	1:G:6175:TYR:HB2	2.07	0.55
1:G:6335:GLN:HA	1:G:6338:GLN:OE1	2.07	0.55
1:B:1427:GLU:N	1:B:1427:GLU:OE1	2.40	0.55
1:C:2089:GLN:HB2	1:C:2096:PHE:CE1	2.42	0.55
1:D:3210:ILE:O	1:D:3214:LYS:HG3	2.06	0.55
1:E:4253:GLN:HG3	1:E:4276:PHE:CZ	2.42	0.55
1:E:4453:LYS:HD3	1:E:4457:GLY:HA2	1.88	0.55
1:F:5477:ALA:CB	1:F:5531:THR:HG22	2.36	0.55
1:G:6338:GLN:HG2	1:G:6339:LYS:N	2.20	0.55
1:G:6408:ALA:HA	1:G:6414:PRO:HG3	1.89	0.55
1:H:7043:GLN:HG3	1:H:7047:MSE:HE3	1.88	0.55
1:H:7376:THR:HG22	1:H:7377:PHE:N	2.22	0.55
1:H:7512:LEU:N	1:H:7512:LEU:CD1	2.70	0.55
1:A:294:ALA:O	1:A:295:GLN:C	2.46	0.55
1:A:476:LEU:O	1:A:476:LEU:HD12	2.07	0.55
1:A:134:PHE:O	1:B:1052:GLY:HA2	2.07	0.55
1:B:1082:TYR:O	1:B:1085:ILE:HG22	2.07	0.55
1:B:1196:ASP:OD1	1:B:1196:ASP:N	2.40	0.55
1:B:1302:ILE:O	1:B:1305:HIS:N	2.40	0.55
1:B:1295:GLN:NE2	1:B:1305:HIS:CE1	2.75	0.55
1:C:2288:LEU:O	1:C:2289:ALA:C	2.46	0.55
1:C:2549:LYS:HA	1:C:2552:TYR:HB3	1.89	0.55
1:D:3269:TYR:HB3	1:D:3273:TYR:CD1	2.42	0.55
1:E:4174:VAL:O	1:E:4174:VAL:HG23	2.06	0.55
1:E:4133:LEU:HB2	1:E:4199:LEU:HD11	1.88	0.55
1:E:4468:VAL:HA	1:E:4471:PHE:CE2	2.42	0.55
1:F:5300:LYS:HD3	1:F:5304:GLU:OE2	2.07	0.55
1:F:5484:ARG:C	1:F:5485:HIS:ND1	2.61	0.55
1:G:6086:MSE:HE2	1:G:6096:PHE:HE1	1.71	0.55
1:G:6165:ARG:NE	1:G:6259:ASN:HD21	2.05	0.55
1:G:6357:LYS:HD2	1:G:6357:LYS:N	2.22	0.55
1:H:7467:ASN:C	1:H:7469:TYR:H	2.10	0.55
1:H:7313:GLY:HA3	3:H:7601:NAD:O5B	2.07	0.55
1:A:154:HIS:O	1:A:197:ARG:HA	2.07	0.54
1:A:506:GLU:O	1:A:511:ARG:HG3	2.08	0.54
1:B:1394:GLY:HA2	1:B:1420:SER:CB	2.36	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2388:THR:HG23	1:C:2415:VAL:CG2	2.37	0.54
1:D:3064:GLN:O	1:D:3067:ARG:HB3	2.06	0.54
1:D:3208:ASP:OD2	1:D:3227:ARG:NH2	2.40	0.54
1:F:5264:ARG:HG3	1:F:5265:PHE:N	2.22	0.54
1:G:6470:ILE:HG22	1:G:6474:VAL:HG21	1.90	0.54
1:H:7086:MSE:HE2	1:H:7096:PHE:HE1	1.72	0.54
1:B:1376:THR:CG2	1:B:1378:GLU:HB3	2.37	0.54
1:B:1381:VAL:HG13	1:B:1407:MSE:CE	2.37	0.54
1:B:1289:ALA:HA	1:B:1499:THR:OG1	2.06	0.54
1:C:2045:ARG:CZ	1:C:2058:ILE:HD13	2.37	0.54
1:C:2522:VAL:O	1:C:2526:ILE:HG13	2.08	0.54
1:F:5212:LEU:C	1:F:5214:LYS:H	2.10	0.54
1:G:6363:GLU:HB2	1:G:6364:PRO:CD	2.37	0.54
1:H:7376:THR:HB	1:H:7379:ASP:OD1	2.07	0.54
1:B:1435:THR:C	1:B:1437:THR:H	2.10	0.54
1:C:2096:PHE:CE2	1:C:2100:LEU:HD23	2.43	0.54
1:C:2122:GLN:O	1:C:2123:TYR:C	2.45	0.54
1:C:2376:THR:HG21	1:C:2378:GLU:HB3	1.88	0.54
1:C:2471:PHE:CG	1:C:2472:PRO:HD3	2.41	0.54
1:C:2499:THR:C	1:C:2501:GLN:N	2.60	0.54
1:D:3381:VAL:O	1:D:3386:PRO:HD3	2.08	0.54
1:E:4315:ALA:HB3	1:E:4392:VAL:CG1	2.37	0.54
1:F:5300:LYS:O	1:F:5302:ILE:N	2.40	0.54
1:F:5317:LEU:N	1:F:5317:LEU:HD12	2.13	0.54
1:F:5550:ALA:O	1:F:5554:LYS:HB2	2.07	0.54
1:G:6374:PRO:HB3	1:G:6383:ILE:HD12	1.88	0.54
1:G:6391:GLY:N	1:G:6417:PHE:O	2.37	0.54
1:G:6108:MSE:HE1	1:G:6519:ILE:HG21	1.88	0.54
1:H:7150:TRP:CD2	1:H:7151:PRO:HD2	2.42	0.54
1:H:7306:LYS:O	1:H:7386:PRO:HA	2.08	0.54
1:H:7309:PHE:HB2	1:H:7343:MSE:CG	2.38	0.54
1:A:270:ARG:CG	1:A:271:GLU:HG2	2.37	0.54
1:A:309:PHE:HD2	1:A:343:MSE:CG	2.20	0.54
1:B:1104:ILE:HG13	1:B:1108:MSE:CE	2.38	0.54
1:B:1156:LYS:HB3	1:B:1479:ILE:HD12	1.89	0.54
1:B:1232:ASP:O	1:B:1235:ILE:N	2.40	0.54
1:D:3140:ARG:NH1	1:D:3230:GLN:HG2	2.22	0.54
1:D:3164:GLU:O	1:D:3171:ASP:N	2.41	0.54
1:D:3253:GLN:HG3	1:D:3276:PHE:CZ	2.42	0.54
1:H:7322:LEU:HD11	1:H:7492:LEU:HB2	1.90	0.54
1:A:301:PRO:O	1:A:302:ILE:C	2.46	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:GLY:O	1:A:315:ALA:N	2.41	0.54
1:B:1075:MSE:CG	1:B:1080:GLU:HG2	2.37	0.54
1:B:1342:TRP:HZ3	1:B:1351:VAL:HG23	1.72	0.54
1:C:2244:ASP:HA	1:C:2248:ARG:HH12	1.72	0.54
1:C:2551:LYS:O	1:C:2551:LYS:HG2	2.08	0.54
1:D:3174:VAL:HG13	1:D:3218:TYR:OH	2.06	0.54
1:D:3133:LEU:HB2	1:D:3199:LEU:HD11	1.89	0.54
1:D:3351:VAL:HG13	1:D:3352:LYS:N	2.22	0.54
1:D:3445:SER:HG	1:D:3449:PHE:HD1	1.56	0.54
1:E:4317:LEU:HD23	1:E:4361:TYR:HB3	1.90	0.54
1:E:4067:ARG:HB2	1:F:5217:PHE:HE1	1.72	0.54
1:H:7301:PRO:O	1:H:7302:ILE:C	2.46	0.54
1:B:1243:THR:CA	1:B:1247:GLY:O	2.56	0.54
1:B:1376:THR:O	1:B:1380:ALA:N	2.39	0.54
1:B:1385:LYS:HB2	1:B:1385:LYS:NZ	2.23	0.54
1:B:1502:LEU:HD21	1:B:1512:LEU:C	2.28	0.54
1:C:2044:GLU:CA	1:C:2048:LEU:HD23	2.37	0.54
1:C:2169:LEU:N	1:C:2169:LEU:HD12	2.23	0.54
1:C:2487:SER:O	1:C:2490:VAL:CG2	2.54	0.54
1:D:3177:MSE:O	1:D:3177:MSE:HE3	2.08	0.54
1:D:3285:ALA:HB1	1:D:3495:ALA:HB2	1.89	0.54
1:D:3494:ALA:O	1:D:3497:ALA:HB3	2.07	0.54
1:F:5103:ASP:HB3	1:F:5107:LEU:CD2	2.38	0.54
1:F:5146:ILE:O	1:F:5149:ASN:HB2	2.08	0.54
1:F:5188:THR:HG23	1:F:5195:PRO:HD3	1.90	0.54
1:F:5559:ARG:HH11	1:F:5559:ARG:HG3	1.72	0.54
1:G:6086:MSE:HE2	1:G:6096:PHE:CE1	2.42	0.54
1:G:6154:HIS:HB3	1:G:6197:ARG:HD3	1.89	0.54
1:G:6223:GLN:HG2	1:G:6224:LYS:O	2.08	0.54
1:G:6313:GLY:O	3:G:6601:NAD:O2N	2.26	0.54
1:G:6376:THR:HG21	1:G:6378:GLU:OE2	2.07	0.54
1:G:6515:PRO:HG2	1:G:6518:ASN:OD1	2.08	0.54
1:H:7176:GLY:O	1:H:7178:GLY:N	2.41	0.54
1:A:210:ILE:O	1:A:213:LEU:HB2	2.08	0.54
1:A:308:LEU:HD12	1:A:309:PHE:H	1.72	0.54
1:A:416:ILE:HD13	1:A:416:ILE:N	2.23	0.54
1:B:1281:GLN:HB3	1:B:1491:PHE:CD2	2.43	0.54
1:B:1325:MSE:O	1:B:1328:VAL:HB	2.07	0.54
1:B:1312:ALA:CB	1:B:1343:MSE:HE3	2.38	0.54
1:C:2177:MSE:HE1	1:C:2200:PRO:HB2	1.90	0.54
1:C:2269:TYR:HB3	1:C:2273:TYR:HD1	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2469:TYR:C	1:C:2470:ILE:HD13	2.28	0.54
1:D:3184:LEU:HG	1:D:3198:CYS:HB3	1.90	0.54
1:D:3391:GLY:HA3	1:D:3427:GLU:CD	2.28	0.54
1:E:4327:MSE:HE1	1:E:4337:ALA:O	2.07	0.54
1:G:6179:ILE:HB	1:G:6180:PRO:HD3	1.89	0.54
1:H:7439:GLY:HA2	1:H:7460:PHE:HE2	1.72	0.54
1:A:339:LYS:HA	1:A:367:HIS:CE1	2.43	0.54
1:A:41:THR:O	1:A:45:ARG:HG3	2.07	0.54
1:B:1302:ILE:HA	1:B:1305:HIS:CE1	2.43	0.54
1:D:3351:VAL:CG2	1:D:3369:ALA:HA	2.35	0.54
1:D:3043:GLN:CG	1:D:3566:LEU:HD11	2.33	0.54
1:F:5467:ASN:C	1:F:5469:TYR:N	2.61	0.54
1:G:6137:ILE:HG22	1:G:6221:LEU:HD23	1.88	0.54
1:G:6404:ILE:HD13	1:G:6436:LEU:HD22	1.90	0.54
1:A:194:ARG:CB	1:A:197:ARG:HG3	2.38	0.54
1:A:505:GLU:N	1:A:505:GLU:OE2	2.36	0.54
1:B:1184:LEU:HD23	1:B:1200:PRO:CG	2.38	0.54
1:B:1416:ILE:H	1:B:1416:ILE:HD13	1.72	0.54
1:C:2133:LEU:HB3	1:C:2201:VAL:HG22	1.90	0.54
1:C:2243:THR:HB	1:C:2248:ARG:CZ	2.38	0.54
1:C:2271:GLU:HA	1:C:2485:HIS:HD2	1.73	0.54
1:C:2546:PRO:HD2	1:C:2549:LYS:HE3	1.90	0.54
1:E:4072:LEU:HD11	1:E:4081:LYS:HB3	1.90	0.54
1:E:4389:ILE:HG22	1:E:4416:ILE:HA	1.89	0.54
1:F:5147:VAL:O	1:F:5245:ARG:NH1	2.40	0.54
1:F:5416:ILE:HD11	1:F:5443:PHE:HB2	1.90	0.54
1:G:6232:ASP:OD2	1:G:6232:ASP:N	2.30	0.54
1:A:236:ASP:O	1:A:239:MSE:N	2.41	0.54
1:A:350:LEU:HD22	1:A:354:ARG:HH12	1.72	0.54
1:A:534:LEU:HA	1:A:539:MSE:HG3	1.89	0.54
1:C:2179:ILE:HB	1:C:2180:PRO:CD	2.37	0.54
1:C:2197:ARG:HH11	1:C:2197:ARG:CG	1.98	0.54
1:C:2333:SER:O	1:C:2334:GLU:C	2.47	0.54
1:C:2418:ALA:HB1	1:C:2427:GLU:H	1.73	0.54
1:D:3227:ARG:HH11	1:D:3227:ARG:HG2	1.72	0.54
1:D:3275:THR:C	1:D:3486:ILE:HD11	2.28	0.54
1:D:3553:VAL:C	1:D:3555:GLU:H	2.11	0.54
1:E:4046:GLN:HG3	1:E:4051:GLN:HG3	1.90	0.54
1:E:4206:GLY:N	1:E:4223:GLN:HE21	2.05	0.54
1:F:5059:GLU:HG2	1:F:5063:ILE:HG21	1.90	0.54
1:F:5105:GLU:OE1	1:F:5517:ALA:HB2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:5177:MSE:CE	1:F:5181:VAL:HG23	2.38	0.54
1:F:5253:GLN:NE2	1:F:5255:GLU:HG2	2.23	0.54
1:G:6359:ASP:O	1:G:6363:GLU:OE1	2.26	0.54
1:H:7104:ILE:O	1:H:7108:MSE:HB2	2.08	0.54
1:H:7308:LEU:O	1:H:7389:ILE:CD1	2.56	0.54
1:A:146:ILE:HD12	1:A:146:ILE:H	1.72	0.53
1:A:295:GLN:OE1	1:A:305:HIS:NE2	2.39	0.53
1:A:527:ALA:O	1:A:531:THR:CG2	2.52	0.53
1:A:566:LEU:HD23	1:A:567:PRO:HD2	1.89	0.53
1:B:1206:GLY:HA3	1:B:1223:GLN:NE2	2.23	0.53
1:B:1319:ILE:HG22	1:B:1323:ILE:HD11	1.89	0.53
1:B:1298:ILE:HD12	1:B:1413:ARG:HD3	1.90	0.53
1:C:2277:ASN:OD1	1:C:2277:ASN:C	2.47	0.53
1:D:3300:LYS:O	1:D:3302:ILE:N	2.41	0.53
1:D:3421:ASN:HB2	3:D:3601:NAD:O2D	2.06	0.53
1:E:4137:ILE:HG13	1:E:4137:ILE:O	2.07	0.53
1:E:4332:LEU:HD23	1:E:4337:ALA:CA	2.38	0.53
1:E:4502:LEU:CD1	1:E:4506:GLU:HB3	2.37	0.53
1:F:5048:LEU:CD2	1:F:5048:LEU:N	2.70	0.53
1:F:5349:LEU:HD23	1:F:5351:VAL:HB	1.90	0.53
1:A:177:MSE:SE	1:A:202:CYS:HB2	2.58	0.53
1:B:1347:TYR:HB3	1:B:1356:ALA:CB	2.38	0.53
1:B:1322:LEU:HG	1:B:1492:LEU:HB2	1.90	0.53
1:B:1101:GLN:HB3	1:B:1520:GLN:HE22	1.73	0.53
1:C:2503:THR:O	1:C:2507:LEU:CD2	2.56	0.53
1:D:3300:LYS:HB3	1:D:3304:GLU:OE2	2.07	0.53
1:D:3337:ALA:C	1:D:3339:LYS:H	2.11	0.53
1:E:4225:ARG:CG	1:E:4225:ARG:NH1	2.69	0.53
1:E:4279:ASP:OD1	1:E:4279:ASP:N	2.32	0.53
1:E:4327:MSE:O	1:E:4330:ASN:HB2	2.08	0.53
1:F:5169:LEU:N	1:F:5169:LEU:CD1	2.71	0.53
1:G:6061:GLN:OE1	1:G:6098:ARG:HD3	2.07	0.53
1:H:7261:ASN:N	1:H:7261:ASN:ND2	2.56	0.53
1:H:7469:TYR:OH	1:H:7516:LEU:HD12	2.07	0.53
1:A:104:ILE:HG23	1:A:105:GLU:N	2.24	0.53
1:A:306:LYS:HB3	1:A:386:PRO:HA	1.89	0.53
1:C:2266:LEU:HD21	1:C:2281:GLN:NE2	2.22	0.53
1:C:2308:LEU:O	1:C:2389:ILE:HD12	2.08	0.53
1:C:2420:SER:HB3	1:C:2425:GLN:HB3	1.91	0.53
1:D:3527:ALA:O	1:D:3531:THR:HG23	2.09	0.53
1:E:4174:VAL:HG11	1:E:4220:GLY:CA	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:5309:PHE:CD1	1:F:5390:ILE:HB	2.42	0.53
1:G:6089:GLN:OE1	1:G:6131:LYS:NZ	2.42	0.53
1:G:6306:LYS:HD2	1:G:6386:PRO:HA	1.91	0.53
1:H:7489:SER:HB2	1:H:7533:TYR:OH	2.07	0.53
1:A:255:GLU:O	1:A:256:ASP:C	2.47	0.53
1:B:1186:LEU:O	1:B:1187:TYR:C	2.47	0.53
1:D:3196:ASP:OD1	1:D:3196:ASP:N	2.40	0.53
1:E:4128:ARG:HH11	1:E:4128:ARG:HG2	1.74	0.53
1:E:4425:GLN:NE2	1:E:4425:GLN:N	2.56	0.53
1:E:4515:PRO:C	1:E:4517:ALA:H	2.11	0.53
1:F:5303:SER:CA	1:F:5340:LYS:HZ2	2.16	0.53
1:F:5379:ASP:O	1:F:5383:ILE:HG13	2.08	0.53
1:E:4567:PRO:HG3	1:G:6047:MSE:HG3	1.89	0.53
1:G:6301:PRO:O	1:G:6303:SER:N	2.42	0.53
1:G:6332:LEU:HD23	1:G:6337:ALA:HA	1.90	0.53
1:G:6381:VAL:CG1	1:G:6407:MSE:HE1	2.38	0.53
1:H:7029:MSE:HE1	1:H:7053:LEU:HD13	1.90	0.53
1:A:267:ARG:HD2	1:A:361:TYR:OH	2.08	0.53
1:B:1035:ASN:OD1	1:B:1036:LYS:N	2.41	0.53
1:B:1103:ASP:HB3	1:B:1107:LEU:HD23	1.91	0.53
1:A:66:LEU:HD23	1:B:1217:PHE:CZ	2.43	0.53
1:D:3280:ILE:HG13	1:D:3314:GLU:OE2	2.08	0.53
1:E:4487:SER:O	1:E:4490:VAL:HG23	2.09	0.53
1:G:6332:LEU:HD23	1:G:6337:ALA:CA	2.38	0.53
1:G:6420:SER:HB3	1:G:6425:GLN:HB3	1.90	0.53
1:H:7553:VAL:C	1:H:7555:GLU:H	2.11	0.53
1:B:1420:SER:HB2	1:B:1427:GLU:OE1	2.09	0.53
1:B:1397:ARG:NH1	1:B:1429:THR:HG22	2.24	0.53
1:C:2154:HIS:O	1:C:2197:ARG:HD2	2.08	0.53
1:C:2417:PHE:CD2	1:C:2444:ALA:HB3	2.43	0.53
1:D:3352:LYS:CG	1:D:3368:SER:HA	2.39	0.53
1:D:3482:ASN:ND2	1:D:3482:ASN:N	2.56	0.53
1:E:4024:LYS:O	1:E:4027:PRO:HD2	2.08	0.53
1:G:6108:MSE:SE	1:G:6468:VAL:HG21	2.58	0.53
1:H:7232:ASP:N	1:H:7232:ASP:OD2	2.41	0.53
1:A:302:ILE:HA	1:A:305:HIS:CE1	2.44	0.53
1:B:1167:LEU:C	1:B:1169:LEU:H	2.12	0.53
1:B:1283:THR:O	1:B:1284:ALA:C	2.47	0.53
1:B:1416:ILE:HD12	1:B:1441:CYS:HB2	1.91	0.53
1:D:3239:MSE:SE	1:D:3252:ILE:HG21	2.57	0.53
1:D:3183:LYS:NZ	1:D:3255:GLU:OE2	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3351:VAL:HG11	1:D:3369:ALA:HB2	1.90	0.53
1:E:4308:LEU:HD12	1:E:4309:PHE:H	1.74	0.53
1:F:5300:LYS:NZ	1:F:5304:GLU:HB2	2.24	0.53
1:G:6042:LEU:O	1:G:6045:ARG:HB2	2.08	0.53
1:G:6207:THR:OG1	1:G:6208:ASP:N	2.41	0.53
1:H:7245:ARG:HD3	1:H:7246:TYR:CE1	2.43	0.53
1:A:370:PRO:HG2	1:A:372:SER:O	2.09	0.53
1:B:1262:ALA:O	1:B:1266:LEU:HB2	2.09	0.53
1:B:1440:ARG:HB3	1:B:1440:ARG:NH1	2.24	0.53
1:B:1470:ILE:C	1:B:1472:PRO:HD2	2.29	0.53
1:C:2086:MSE:CE	1:C:2111:VAL:HG13	2.39	0.53
1:C:2175:TYR:CD2	1:C:2219:MSE:HE2	2.44	0.53
1:C:2439:GLY:CA	1:C:2460:PHE:HE2	2.13	0.53
1:D:3060:THR:O	1:D:3064:GLN:HG3	2.09	0.53
1:D:3193:ILE:HG22	1:D:3194:ARG:N	2.23	0.53
1:D:3389:ILE:HG23	1:D:3399:PHE:CE1	2.44	0.53
1:E:4363:GLU:HA	1:E:4366:THR:OG1	2.09	0.53
1:E:4437:THR:O	1:E:4439:GLY:N	2.42	0.53
1:F:5026:LYS:N	1:F:5027:PRO:HD2	2.24	0.53
1:G:6245:ARG:HG2	1:G:6246:TYR:CD1	2.43	0.53
1:G:6390:ILE:HG23	1:G:6419:LEU:HD21	1.91	0.53
1:H:7127:PHE:CD2	1:H:7128:ARG:N	2.77	0.53
1:H:7244:ASP:N	1:H:7248:ARG:HH11	2.05	0.53
1:H:7553:VAL:C	1:H:7555:GLU:N	2.62	0.53
1:A:66:LEU:HD23	1:B:1217:PHE:HZ	1.74	0.53
1:B:1254:PHE:O	1:B:1255:GLU:HG2	2.08	0.53
1:C:2381:VAL:HG22	1:C:2407:MSE:HE1	1.90	0.53
1:D:3295:GLN:HG3	1:D:3295:GLN:O	2.09	0.53
1:D:3301:PRO:O	1:D:3302:ILE:C	2.46	0.53
1:E:4218:TYR:O	1:F:5057:LYS:NZ	2.40	0.53
1:E:4253:GLN:NE2	1:E:4278:ASP:HB2	2.23	0.53
1:F:5418:ALA:O	1:F:5445:SER:HA	2.09	0.53
1:H:7059:GLU:HA	1:H:7063:ILE:HD12	1.91	0.53
1:H:7302:ILE:HG22	1:H:7303:SER:N	2.24	0.53
1:H:7508:ALA:O	1:H:7509:GLN:C	2.48	0.53
1:A:108:MSE:HB3	1:A:109:PRO:HD3	1.89	0.53
1:A:261:ASN:HB3	1:A:265:PHE:CE1	2.44	0.53
1:B:1159:VAL:HG11	1:B:1180:PRO:HA	1.91	0.53
1:B:1288:LEU:CD1	1:B:1323:ILE:HA	2.39	0.53
1:C:2402:ASP:HA	1:C:2405:ARG:HD2	1.91	0.53
1:C:2528:ILE:O	1:C:2530:VAL:N	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3302:ILE:HA	1:D:3305:HIS:ND1	2.24	0.53
1:D:3454:LEU:HD13	1:D:3458:ARG:NH1	2.24	0.53
1:E:4166:ILE:HA	1:E:4256:ASP:OD1	2.09	0.53
1:E:4359:ASP:OD2	1:E:4359:ASP:C	2.46	0.53
1:G:6297:VAL:CG2	1:G:6298:ILE:N	2.71	0.53
1:G:6291:LEU:HD23	1:G:6417:PHE:CE2	2.44	0.53
1:G:6217:PHE:CE1	1:H:7067:ARG:HB2	2.42	0.53
1:H:7295:GLN:HA	1:H:7298:ILE:HB	1.89	0.53
1:A:319:ILE:O	1:A:321:ASN:N	2.43	0.52
1:B:1274:CYS:SG	1:B:1478:VAL:HG11	2.49	0.52
1:B:1416:ILE:HG12	1:B:1443:PHE:HD1	1.74	0.52
1:C:2045:ARG:HA	1:C:2050:LEU:HB2	1.91	0.52
1:C:2144:ARG:O	1:C:2148:ASP:OD2	2.27	0.52
1:C:2453:LYS:CE	1:C:2457:GLY:HA2	2.39	0.52
1:C:2458:ARG:HH11	1:C:2458:ARG:CB	2.22	0.52
1:A:42:LEU:HD21	1:C:2572:TRP:HB2	1.91	0.52
1:D:3351:VAL:HA	1:D:3367:HIS:O	2.09	0.52
1:G:6227:ARG:HH11	1:G:6227:ARG:CG	2.22	0.52
1:H:7194:ARG:HB3	1:H:7197:ARG:HG3	1.90	0.52
1:H:7283:THR:HA	1:H:7467:ASN:ND2	2.24	0.52
1:H:7499:THR:C	1:H:7501:GLN:H	2.13	0.52
1:A:156:LYS:N	1:A:197:ARG:O	2.42	0.52
1:A:286:VAL:O	1:A:289:ALA:HB3	2.09	0.52
1:B:1263:PHE:O	1:B:1266:LEU:HB3	2.09	0.52
1:B:1357:LYS:N	1:B:1357:LYS:HD3	2.24	0.52
1:C:2399:PHE:CG	1:C:2427:GLU:HB3	2.45	0.52
1:D:3204:ASP:OD1	1:D:3221:LEU:HD22	2.09	0.52
1:D:3376:THR:HG22	1:D:3378:GLU:HG2	1.88	0.52
1:D:3480:LEU:CD1	1:D:3553:VAL:HG13	2.38	0.52
1:E:4026:LYS:HG3	1:E:4029:MSE:CE	2.39	0.52
1:E:4108:MSE:HB3	1:E:4109:PRO:CD	2.39	0.52
1:E:4402:ASP:O	1:E:4406:ALA:N	2.33	0.52
1:E:4453:LYS:HE3	1:E:4457:GLY:HA2	1.92	0.52
1:F:5531:THR:HA	1:F:5534:LEU:HD12	1.91	0.52
1:G:6351:VAL:HG11	1:G:6369:ALA:HB2	1.91	0.52
1:G:6390:ILE:HG22	1:G:6392:VAL:HG23	1.91	0.52
1:A:171:ASP:O	1:A:172:LEU:HD23	2.09	0.52
1:A:295:GLN:O	1:A:299:SER:N	2.36	0.52
1:A:41:THR:HG23	1:A:44:GLU:CD	2.29	0.52
1:B:1363:GLU:HB2	1:B:1364:PRO:HD3	1.91	0.52
1:D:3396:GLY:HA2	1:D:3425:GLN:HA	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3437:THR:HG21	1:D:3441:CYS:CB	2.23	0.52
1:E:4104:ILE:HG13	1:E:4108:MSE:CE	2.39	0.52
1:F:5031:ASN:HB3	1:F:5034:THR:OG1	2.09	0.52
1:F:5137:ILE:HG23	1:F:5138:SER:N	2.23	0.52
1:F:5480:LEU:HD13	1:F:5553:VAL:HG22	1.92	0.52
1:G:6210:ILE:N	1:G:6213:LEU:HD12	2.23	0.52
1:G:6320:ALA:O	1:G:6323:ILE:HB	2.09	0.52
1:G:6376:THR:HB	1:G:6379:ASP:CG	2.30	0.52
1:H:7258:GLY:O	1:H:7259:ASN:C	2.47	0.52
1:H:7498:LEU:O	1:H:7501:GLN:N	2.43	0.52
1:A:176:GLY:O	1:A:178:GLY:N	2.42	0.52
1:A:269:TYR:HB3	1:A:273:TYR:CD1	2.44	0.52
1:A:347:TYR:HB2	1:A:354:ARG:NH2	2.25	0.52
1:A:503:THR:O	1:A:507:LEU:HD22	2.09	0.52
1:A:518:ASN:O	1:A:521:GLU:HG2	2.10	0.52
1:B:1238:PHE:CE1	1:B:1242:ILE:CG1	2.92	0.52
1:B:1552:TYR:CE1	1:B:1556:ARG:NE	2.77	0.52
1:E:4038:MSE:SE	1:E:4055:PRO:HG2	2.59	0.52
1:A:325:MSE:HE1	1:A:489:SER:HA	1.91	0.52
1:A:531:THR:HA	1:A:534:LEU:HD12	1.91	0.52
1:B:1041:THR:HG23	1:B:1044:GLU:HG3	1.90	0.52
1:B:1123:TYR:C	1:B:1125:HIS:H	2.13	0.52
1:C:2186:LEU:O	1:C:2187:TYR:C	2.47	0.52
1:C:2209:ASN:HB3	1:C:2212:LEU:HB2	1.91	0.52
1:C:2302:ILE:HG22	1:C:2303:SER:N	2.23	0.52
1:E:4041:THR:HG23	1:E:4044:GLU:CG	2.38	0.52
1:E:4335:GLN:HE21	1:E:4339:LYS:HG3	1.74	0.52
1:F:5094:LYS:HD2	1:F:5562:TYR:HA	1.90	0.52
1:G:6341:ILE:O	1:G:6367:HIS:NE2	2.43	0.52
1:G:6505:GLU:O	1:G:6508:ALA:HB3	2.09	0.52
1:H:7112:TYR:CE2	1:H:7113:THR:HG23	2.44	0.52
1:H:7531:THR:O	1:H:7534:LEU:HB2	2.10	0.52
1:A:428:CYS:HG	1:A:429:THR:H	1.55	0.52
1:B:1298:ILE:HD11	1:B:1442:LEU:CD1	2.33	0.52
1:B:1352:LYS:HB2	1:B:1368:SER:HA	1.91	0.52
1:B:1444:ALA:HB2	1:B:1512:LEU:HD13	1.92	0.52
1:B:1447:SER:HB3	1:B:1448:PRO:HD2	1.91	0.52
1:C:2175:TYR:HD2	1:C:2219:MSE:HE2	1.74	0.52
1:C:2257:PHE:HB2	1:C:2262:ALA:HB2	1.92	0.52
1:C:2380:ALA:O	1:C:2381:VAL:C	2.48	0.52
1:C:2569:VAL:CG1	1:C:2570:TYR:N	2.65	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3108:MSE:N	1:D:3109:PRO:CD	2.72	0.52
1:D:3288:LEU:O	1:D:3292:LEU:N	2.42	0.52
1:E:4041:THR:HG23	1:E:4044:GLU:OE1	2.10	0.52
1:E:4350:LEU:HD13	1:E:4354:ARG:CD	2.39	0.52
1:E:4402:ASP:O	1:E:4406:ALA:CB	2.57	0.52
1:G:6133:LEU:HD13	1:G:6150:TRP:CE3	2.44	0.52
1:G:6493:GLU:HA	1:G:6496:LYS:CD	2.34	0.52
1:G:6511:ARG:HB2	1:G:6511:ARG:HH11	1.74	0.52
1:B:1029:MSE:SE	1:B:1050:LEU:HD22	2.59	0.52
1:B:1399:PHE:HA	1:B:1403:VAL:CG1	2.32	0.52
1:B:1542:ARG:HD2	1:B:1552:TYR:OH	2.09	0.52
1:C:2196:ASP:OD1	1:C:2196:ASP:N	2.41	0.52
1:C:2374:PRO:CD	1:C:2383:ILE:HD12	2.39	0.52
1:D:3261:ASN:HD22	1:D:3261:ASN:H	1.55	0.52
1:D:3477:ALA:CB	1:D:3531:THR:HG22	2.34	0.52
1:E:4085:ILE:HA	1:E:4088:ILE:HG12	1.92	0.52
1:E:4515:PRO:C	1:E:4517:ALA:N	2.62	0.52
1:E:4553:VAL:C	1:E:4555:GLU:H	2.13	0.52
1:F:5303:SER:N	1:F:5340:LYS:NZ	2.58	0.52
1:F:5570:TYR:CE1	1:H:7046:GLN:NE2	2.78	0.52
1:G:6290:GLY:O	1:G:6293:ALA:HB3	2.09	0.52
1:G:6492:LEU:CD2	1:G:6496:LYS:HD2	2.40	0.52
1:H:7047:MSE:O	1:H:7048:LEU:HD13	2.10	0.52
1:H:7130:PRO:C	1:H:7131:LYS:HG2	2.30	0.52
1:B:1531:THR:OG1	1:B:1532:GLU:N	2.41	0.52
1:B:1546:PRO:O	1:B:1549:LYS:NZ	2.43	0.52
1:D:3230:GLN:O	1:D:3233:ASP:HB2	2.10	0.52
1:D:3279:ASP:N	1:D:3279:ASP:OD1	2.42	0.52
1:D:3300:LYS:HB2	1:D:3305:HIS:HE2	1.75	0.52
1:D:3302:ILE:O	1:D:3304:GLU:N	2.42	0.52
1:D:3391:GLY:N	1:D:3417:PHE:O	2.42	0.52
1:E:4271:GLU:O	1:E:4485:HIS:NE2	2.42	0.52
1:F:5209:ASN:OD1	1:F:5211:ALA:HB3	2.09	0.52
1:F:5300:LYS:O	1:F:5305:HIS:NE2	2.43	0.52
1:F:5327:MSE:CE	1:F:5341:ILE:HD11	2.40	0.52
1:G:6408:ALA:O	1:G:6411:ASN:O	2.28	0.52
1:G:6298:ILE:HD11	1:G:6413:ARG:HB3	1.92	0.52
1:H:7090:GLU:HG2	1:H:7131:LYS:NZ	2.25	0.52
1:H:7156:LYS:HE2	1:H:7156:LYS:HA	1.92	0.52
1:H:7412:GLU:C	1:H:7413:ARG:HG2	2.29	0.52
1:B:1293:ALA:O	1:B:1296:LYS:HB3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1453:LYS:HB2	1:B:1459:VAL:CG1	2.40	0.52
1:D:3116:VAL:HG13	1:D:3117:GLY:N	2.24	0.52
1:D:3194:ARG:HB3	1:D:3197:ARG:HG2	1.92	0.52
1:D:3243:THR:HG22	1:D:3248:ARG:HA	1.91	0.52
1:E:4113:THR:HB	1:E:4114:PRO:HA	1.90	0.52
1:E:4313:GLY:O	1:E:4315:ALA:N	2.42	0.52
1:F:5144:ARG:NH1	1:F:5244:ASP:CB	2.73	0.52
1:F:5481:CYS:SG	1:F:5531:THR:HB	2.50	0.52
1:G:6143:VAL:O	1:G:6146:ILE:HB	2.09	0.52
1:G:6180:PRO:O	1:G:6184:LEU:HD22	2.10	0.52
1:H:7351:VAL:HG11	1:H:7369:ALA:HB2	1.92	0.52
1:A:123:TYR:O	1:A:175:TYR:CZ	2.62	0.52
1:A:317:LEU:HD23	1:A:361:TYR:O	2.10	0.52
1:A:393:ALA:HA	3:A:601:NAD:O4B	2.10	0.52
1:A:412:GLU:HA	1:A:440:ARG:NH1	2.24	0.52
1:A:394:GLY:HA2	1:A:420:SER:HB3	1.91	0.52
1:A:57:LYS:HG3	1:B:1218:TYR:O	2.10	0.52
1:B:1154:HIS:O	1:B:1197:ARG:HD3	2.09	0.52
1:B:1229:GLN:HG3	1:B:1233:ASP:OD2	2.10	0.52
1:B:1342:TRP:CZ3	1:B:1351:VAL:HG23	2.44	0.52
1:C:2439:GLY:HA3	1:C:2460:PHE:CE2	2.27	0.52
1:D:3418:ALA:HB1	1:D:3427:GLU:HB2	1.90	0.52
1:E:4108:MSE:N	1:E:4109:PRO:HD2	2.25	0.52
1:E:4252:ILE:O	1:E:4275:THR:HA	2.10	0.52
1:F:5142:HIS:O	1:F:5143:VAL:C	2.49	0.52
1:A:261:ASN:N	1:A:261:ASN:ND2	2.58	0.51
1:A:264:ARG:HG3	1:A:265:PHE:H	1.73	0.51
1:A:471:PHE:CD1	1:A:472:PRO:HD3	2.45	0.51
1:B:1350:LEU:HD12	1:B:1366:THR:OG1	2.10	0.51
1:C:2518:ASN:HB3	1:C:2521:GLU:CD	2.31	0.51
1:D:3354:ARG:HG3	1:D:3358:ILE:HD11	1.92	0.51
1:D:3453:LYS:CD	1:D:3457:GLY:HA2	2.40	0.51
1:E:4037:GLY:O	1:E:4039:ALA:N	2.42	0.51
1:E:4344:PHE:HD1	1:E:4349:LEU:HB2	1.75	0.51
1:E:4418:ALA:O	1:E:4445:SER:HA	2.10	0.51
1:E:4310:LEU:HD23	1:E:4427:GLU:HG2	1.91	0.51
1:F:5352:LYS:HG2	1:F:5367:HIS:O	2.10	0.51
1:E:4570:TYR:H	1:G:6046:GLN:HE22	1.58	0.51
1:G:6075:MSE:SE	1:G:6081:LYS:HA	2.61	0.51
1:G:6166:ILE:HA	1:G:6256:ASP:OD1	2.10	0.51
1:G:6302:ILE:HD12	1:G:6302:ILE:N	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:6416:ILE:CD1	1:G:6416:ILE:N	2.73	0.51
1:G:6535:TYR:OH	1:G:6545:GLU:HA	2.10	0.51
1:H:7033:ARG:NH2	1:H:7196:ASP:HA	2.25	0.51
1:H:7143:VAL:O	1:H:7147:VAL:HG23	2.10	0.51
1:H:7453:LYS:HD3	1:H:7454:LEU:O	2.11	0.51
1:H:7519:ILE:O	1:H:7519:ILE:HG13	2.07	0.51
1:H:7551:LYS:O	1:H:7555:GLU:HB2	2.09	0.51
1:A:281:GLN:HE21	1:A:491:PHE:HE1	1.56	0.51
1:A:327:MSE:CE	1:A:337:ALA:HB1	2.31	0.51
1:B:1301:PRO:O	1:B:1302:ILE:C	2.48	0.51
1:B:1454:LEU:HB2	1:B:1456:ASP:OD1	2.11	0.51
1:C:2315:ALA:CB	1:C:2392:VAL:HG11	2.33	0.51
1:D:3389:ILE:C	1:D:3390:ILE:HG13	2.30	0.51
1:D:3494:ALA:O	1:D:3495:ALA:C	2.47	0.51
1:D:3537:ASN:ND2	1:D:3537:ASN:N	2.58	0.51
1:E:4229:GLN:HA	1:E:4229:GLN:OE1	2.10	0.51
1:E:4381:VAL:HG13	1:E:4407:MSE:CE	2.41	0.51
1:E:4487:SER:HB2	1:E:4489:SER:OG	2.10	0.51
1:E:4518:ASN:O	1:E:4522:VAL:HG23	2.10	0.51
1:F:5174:VAL:HG21	1:F:5219:MSE:O	2.10	0.51
1:F:5350:LEU:HD12	1:F:5366:THR:HG23	1.92	0.51
1:F:5392:VAL:O	1:F:5392:VAL:CG1	2.58	0.51
1:G:6097:TYR:O	1:G:6101:GLN:HG3	2.09	0.51
1:H:7116:VAL:HG13	1:H:7117:GLY:H	1.73	0.51
1:A:378:GLU:O	1:A:381:VAL:HB	2.10	0.51
1:B:1482:ASN:N	1:B:1482:ASN:ND2	2.58	0.51
1:C:2541:PHE:CD2	1:C:2541:PHE:N	2.75	0.51
1:D:3086:MSE:HE2	1:D:3086:MSE:HA	1.92	0.51
1:D:3276:PHE:HB3	1:D:3486:ILE:CD1	2.39	0.51
1:D:3308:LEU:HB3	1:D:3389:ILE:HD12	1.92	0.51
1:D:3372:SER:O	1:D:3383:ILE:HG21	2.09	0.51
1:E:4123:TYR:HD2	1:E:4219:MSE:CE	2.23	0.51
1:E:4338:GLN:O	1:E:4367:HIS:CE1	2.64	0.51
1:E:4530:VAL:HG12	1:E:4534:LEU:CD1	2.37	0.51
1:F:5176:GLY:O	1:F:5178:GLY:N	2.43	0.51
1:G:6359:ASP:C	1:G:6359:ASP:OD2	2.48	0.51
1:G:6429:THR:O	1:G:6430:ALA:C	2.49	0.51
1:G:6453:LYS:HA	1:G:6458:ARG:O	2.09	0.51
1:H:7024:LYS:O	1:H:7027:PRO:HD2	2.08	0.51
1:H:7351:VAL:CG2	1:H:7369:ALA:HA	2.41	0.51
1:H:7376:THR:CG2	1:H:7377:PHE:N	2.73	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:ALA:HA	1:A:322:LEU:CD2	2.40	0.51
1:A:499:THR:C	1:A:501:GLN:H	2.14	0.51
1:A:512:LEU:CD1	1:A:512:LEU:N	2.70	0.51
1:B:1325:MSE:HE2	1:B:1492:LEU:HD13	1.92	0.51
1:B:1351:VAL:HG13	1:B:1352:LYS:N	2.25	0.51
1:B:1471:PHE:CD1	1:B:1472:PRO:HD3	2.46	0.51
1:C:2024:LYS:HA	1:C:2028:LEU:HD22	1.92	0.51
1:C:2244:ASP:CA	1:C:2248:ARG:HH12	2.23	0.51
1:C:2419:LEU:CD2	1:C:2419:LEU:H	2.20	0.51
1:C:2432:GLU:HA	1:C:2436:LEU:CD1	2.35	0.51
1:C:2524:ILE:O	1:C:2528:ILE:HG12	2.11	0.51
1:D:3107:LEU:O	1:D:3111:VAL:HG23	2.11	0.51
1:E:4350:LEU:HD12	1:E:4366:THR:HG23	1.91	0.51
1:F:5082:TYR:O	1:F:5085:ILE:HG22	2.10	0.51
1:H:7156:LYS:O	1:H:7251:LEU:HB3	2.10	0.51
1:H:7243:THR:HB	1:H:7248:ARG:CD	2.32	0.51
1:A:413:ARG:NH2	1:A:440:ARG:C	2.64	0.51
1:B:1332:LEU:HG	1:B:1336:GLU:OE2	2.10	0.51
1:C:2051:GLN:HA	1:C:2051:GLN:NE2	2.19	0.51
1:D:3047:MSE:O	1:D:3048:LEU:HD22	2.10	0.51
1:D:3133:LEU:HD12	1:D:3134:PHE:H	1.75	0.51
1:E:4128:ARG:HG2	1:E:4128:ARG:NH1	2.26	0.51
1:E:4359:ASP:OD2	1:E:4361:TYR:N	2.44	0.51
1:E:4416:ILE:O	1:E:4417:PHE:HD1	1.93	0.51
1:F:5408:ALA:CB	1:F:5437:THR:HG22	2.37	0.51
1:G:6342:TRP:CD2	1:G:6384:LEU:HD21	2.45	0.51
1:G:6453:LYS:HG3	1:G:6459:VAL:HG13	1.93	0.51
1:H:7407:MSE:CG	1:H:7414:PRO:HB2	2.38	0.51
1:H:7389:ILE:CG2	1:H:7416:ILE:HG22	2.40	0.51
1:A:120:CYS:O	1:A:175:TYR:HB3	2.11	0.51
1:A:407:MSE:HG3	1:A:414:PRO:HB2	1.92	0.51
1:B:1264:ARG:CG	1:B:1265:PHE:N	2.73	0.51
1:C:2082:TYR:CD2	1:C:2082:TYR:C	2.84	0.51
1:C:2518:ASN:HB3	1:C:2521:GLU:OE2	2.11	0.51
1:D:3095:LEU:O	1:D:3096:PHE:C	2.47	0.51
1:D:3454:LEU:HD11	1:D:3460:PHE:HE2	1.75	0.51
1:E:4511:ARG:HH11	1:E:4511:ARG:CB	2.24	0.51
1:G:6144:ARG:O	1:G:6148:ASP:OD2	2.28	0.51
1:G:6467:ASN:O	1:G:6469:TYR:N	2.44	0.51
1:H:7315:ALA:O	1:H:7319:ILE:HG13	2.09	0.51
1:H:7407:MSE:HA	1:H:7407:MSE:HE2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:7531:THR:O	1:H:7534:LEU:N	2.43	0.51
1:A:342:TRP:CE2	1:A:367:HIS:HD2	2.29	0.51
1:A:344:PHE:CZ	1:A:348:GLY:HA2	2.46	0.51
1:A:326:SER:HB2	1:A:492:LEU:HD11	1.93	0.51
1:C:2259:ASN:O	1:C:2260:HIS:C	2.49	0.51
1:D:3063:ILE:O	1:D:3066:LEU:HB3	2.11	0.51
1:D:3109:PRO:O	1:D:3114:PRO:HD2	2.11	0.51
1:D:3187:TYR:O	1:D:3191:ALA:HB3	2.10	0.51
1:D:3135:ILE:O	1:D:3203:ILE:HA	2.10	0.51
1:D:3350:LEU:HD12	1:D:3366:THR:HG23	1.92	0.51
1:D:3389:ILE:HG23	1:D:3399:PHE:CZ	2.46	0.51
1:D:3512:LEU:N	1:D:3512:LEU:HD12	2.26	0.51
1:D:3528:ILE:O	1:D:3532:GLU:HG2	2.11	0.51
1:F:5099:ILE:O	1:F:5102:ASP:HB2	2.10	0.51
1:F:5418:ALA:C	1:F:5419:LEU:HD13	2.31	0.51
1:G:6092:ASN:ND2	1:G:6562:TYR:OH	2.36	0.51
1:H:7127:PHE:C	1:H:7127:PHE:CD2	2.84	0.51
1:H:7172:LEU:O	1:H:7175:TYR:HB2	2.11	0.51
1:H:7522:VAL:O	1:H:7526:ILE:CG1	2.59	0.51
1:A:399:PHE:CG	1:A:427:GLU:HB3	2.46	0.51
1:A:39:ALA:HA	1:A:59:GLU:O	2.11	0.51
1:A:570:TYR:CE2	1:D:3142:HIS:CG	2.98	0.51
1:A:67:ARG:HB2	1:B:1217:PHE:CE1	2.46	0.51
1:B:1232:ASP:CA	1:B:1235:ILE:HG12	2.40	0.51
1:C:2075:MSE:HB3	1:C:2081:LYS:HG2	1.91	0.51
1:C:2283:THR:O	1:C:2286:VAL:HG23	2.10	0.51
1:C:2512:LEU:HD12	1:C:2512:LEU:N	2.26	0.51
1:D:3103:ASP:O	1:D:3107:LEU:HB2	2.10	0.51
1:D:3167:LEU:HB2	1:D:3169:LEU:HD13	1.92	0.51
1:H:7028:LEU:CD2	1:H:7048:LEU:HG	2.41	0.51
1:A:89:GLN:C	1:A:91:ARG:N	2.64	0.51
1:B:1145:SER:HA	1:B:1148:ASP:OD2	2.11	0.51
1:B:1259:ASN:O	1:B:1260:HIS:C	2.49	0.51
1:B:1350:LEU:HA	1:B:1354:ARG:HD3	1.93	0.51
1:B:1454:LEU:HD12	1:B:1458:ARG:CB	2.39	0.51
1:C:2057:LYS:CE	1:C:2059:GLU:HG2	2.41	0.51
1:C:2180:PRO:HB2	1:C:2200:PRO:HB2	1.93	0.51
1:C:2352:LYS:HG3	1:C:2368:SER:CA	2.41	0.51
1:D:3291:LEU:N	1:D:3291:LEU:HD23	2.26	0.51
1:D:3335:GLN:HE21	1:D:3335:GLN:HA	1.76	0.51
1:D:3420:SER:OG	1:D:3427:GLU:OE2	2.27	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:4389:ILE:HG23	1:E:4399:PHE:CE1	2.46	0.51
1:F:5047:MSE:HE3	1:F:5566:LEU:CD2	2.41	0.51
1:F:5324:VAL:HG13	1:F:5337:ALA:CB	2.41	0.51
1:G:6043:GLN:HG2	1:G:6566:LEU:CD1	2.35	0.51
1:G:6104:ILE:HG23	1:G:6105:GLU:N	2.26	0.51
1:G:6030:LEU:O	1:H:7030:LEU:HD13	2.11	0.51
1:H:7402:ASP:O	1:H:7405:ARG:HG2	2.10	0.51
1:A:309:PHE:CD1	1:A:390:ILE:HB	2.41	0.51
1:A:553:VAL:O	1:A:556:ARG:N	2.43	0.51
1:B:1543:TYR:C	1:B:1543:TYR:CD2	2.84	0.51
1:C:2261:ASN:HA	1:C:2264:ARG:HG2	1.93	0.51
1:C:2275:THR:O	1:C:2486:ILE:HG13	2.11	0.51
1:C:2300:LYS:HG2	1:C:2304:GLU:OE1	2.10	0.51
1:C:2549:LYS:O	1:C:2552:TYR:HB3	2.10	0.51
1:D:3109:PRO:HA	1:D:3113:THR:O	2.11	0.51
1:D:3122:GLN:O	1:D:3123:TYR:O	2.28	0.51
1:D:3405:ARG:O	1:D:3408:ALA:HB3	2.11	0.51
1:D:3418:ALA:CB	1:D:3427:GLU:HB2	2.40	0.51
1:E:4515:PRO:O	1:E:4517:ALA:N	2.44	0.51
1:G:6124:GLY:N	4:G:8062:HOH:O	2.45	0.51
1:G:6263:PHE:O	1:G:6266:LEU:HB3	2.11	0.51
1:H:7026:LYS:O	1:H:7029:MSE:N	2.43	0.51
1:A:501:GLN:CA	1:A:501:GLN:HE21	2.24	0.50
1:B:1097:TYR:O	1:B:1098:ARG:C	2.50	0.50
1:B:1251:LEU:HD12	1:B:1252:ILE:H	1.75	0.50
1:C:2045:ARG:NH1	1:C:2058:ILE:HD13	2.25	0.50
1:C:2124:GLY:O	1:C:2217:PHE:HB3	2.11	0.50
1:C:2428:CYS:HG	1:C:2429:THR:N	2.08	0.50
1:C:2298:ILE:CD1	1:C:2442:LEU:HD11	2.38	0.50
1:B:1139:ASP:OD1	1:C:2572:TRP:NE1	2.44	0.50
1:D:3300:LYS:NZ	1:D:3305:HIS:HA	2.24	0.50
1:D:3341:ILE:HD12	1:D:3365:PHE:HE2	1.76	0.50
1:D:3389:ILE:O	1:D:3390:ILE:HG13	2.12	0.50
1:D:3402:ASP:HA	1:D:3405:ARG:CG	2.40	0.50
1:D:3549:LYS:HA	1:D:3552:TYR:HB3	1.92	0.50
1:E:4205:VAL:O	1:E:4225:ARG:HA	2.11	0.50
1:E:4352:LYS:CG	1:E:4368:SER:HA	2.39	0.50
1:E:4476:LEU:HG	1:E:4480:LEU:HD12	1.93	0.50
1:F:5089:GLN:HB2	1:F:5096:PHE:CE1	2.46	0.50
1:F:5103:ASP:HB3	1:F:5107:LEU:HD22	1.92	0.50
1:F:5358:ILE:HG12	1:F:5366:THR:HG21	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:5402:ASP:CA	1:F:5405:ARG:HG2	2.41	0.50
1:F:5467:ASN:C	1:F:5469:TYR:H	2.14	0.50
1:F:5532:GLU:HG2	1:F:5549:LYS:HG2	1.94	0.50
1:G:6024:LYS:O	1:G:6027:PRO:HD2	2.11	0.50
1:G:6183:LYS:O	1:G:6187:TYR:HD1	1.93	0.50
1:G:6205:VAL:HG12	1:G:6226:ASP:CB	2.26	0.50
1:G:6153:ASN:O	1:G:6246:TYR:CE2	2.63	0.50
1:G:6270:ARG:NH2	1:G:6486:ILE:O	2.42	0.50
1:H:7040:PHE:HE2	1:H:7565:LEU:HD12	1.76	0.50
1:H:7389:ILE:HD12	1:H:7390:ILE:H	1.75	0.50
1:E:4138:SER:O	1:H:7572:TRP:NE1	2.44	0.50
1:A:195:PRO:C	1:A:197:ARG:H	2.13	0.50
1:A:217:PHE:HZ	1:B:1066:LEU:HG	1.75	0.50
1:A:408:ALA:O	1:A:440:ARG:NH2	2.40	0.50
1:B:1235:ILE:HG13	1:B:1265:PHE:CZ	2.46	0.50
1:C:2327:MSE:HE2	1:C:2341:ILE:HD11	1.93	0.50
1:C:2545:GLU:HG3	1:C:2546:PRO:HD2	1.92	0.50
1:C:2038:MSE:HE1	1:D:3219:MSE:HG2	1.94	0.50
1:E:4177:MSE:CE	1:E:4181:VAL:HG22	2.39	0.50
1:F:5172:LEU:O	1:F:5175:TYR:HB2	2.11	0.50
1:F:5489:SER:HG	1:F:5533:TYR:HH	1.55	0.50
1:G:6284:ALA:O	1:G:6287:ALA:N	2.44	0.50
1:G:6332:LEU:HG	1:G:6336:GLU:HG3	1.93	0.50
1:H:7135:ILE:HB	1:H:7203:ILE:HG12	1.93	0.50
1:A:100:LEU:HD11	1:A:111:VAL:HG21	1.92	0.50
1:A:144:ARG:NH1	1:A:244:ASP:HB3	2.25	0.50
1:A:245:ARG:O	1:A:245:ARG:HG3	2.09	0.50
1:A:379:ASP:O	1:A:383:ILE:HG13	2.12	0.50
1:C:2057:LYS:HE3	1:C:2059:GLU:HG2	1.93	0.50
1:C:2124:GLY:HA3	1:C:2175:TYR:CE2	2.45	0.50
1:C:2245:ARG:HG2	1:C:2246:TYR:CE1	2.47	0.50
1:C:2440:ARG:HB3	1:C:2440:ARG:NH1	2.27	0.50
1:D:3090:GLU:CG	1:D:3131:LYS:HE2	2.41	0.50
1:D:3154:HIS:O	1:D:3197:ARG:HD3	2.11	0.50
1:D:3482:ASN:O	1:D:3541:PHE:HB2	2.11	0.50
1:D:3535:TYR:O	1:D:3538:LYS:NZ	2.45	0.50
1:E:4099:ILE:O	1:E:4102:ASP:CB	2.60	0.50
1:E:4254:PHE:HD2	1:E:4257:PHE:CE1	2.28	0.50
1:F:5207:THR:O	1:F:5224:LYS:HA	2.12	0.50
1:G:6137:ILE:HA	1:G:6234:LEU:CD2	2.42	0.50
1:H:7278:ASP:O	1:H:7280:ILE:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:7308:LEU:O	1:H:7389:ILE:HD12	2.11	0.50
1:H:7551:LYS:HE3	1:H:7555:GLU:OE1	2.12	0.50
1:B:1061:GLN:OE1	1:B:1098:ARG:HD3	2.10	0.50
1:B:1108:MSE:HB3	1:B:1109:PRO:HD3	1.93	0.50
1:B:1164:GLU:O	1:B:1171:ASP:N	2.44	0.50
1:C:2295:GLN:HA	1:C:2298:ILE:HB	1.93	0.50
1:D:3350:LEU:HD21	1:D:3354:ARG:HH22	1.77	0.50
1:E:4154:HIS:HB3	1:E:4197:ARG:CD	2.42	0.50
1:E:4333:SER:O	1:E:4335:GLN:N	2.44	0.50
1:F:5381:VAL:O	1:F:5386:PRO:HD3	2.12	0.50
1:F:5401:PRO:O	1:F:5405:ARG:HG2	2.11	0.50
1:G:6298:ILE:CG2	1:G:6300:LYS:HB2	2.41	0.50
1:H:7072:LEU:HD11	1:H:7081:LYS:HB3	1.94	0.50
1:H:7104:ILE:HG13	1:H:7108:MSE:HE1	1.94	0.50
1:H:7481:CYS:HB3	1:H:7483:THR:OG1	2.12	0.50
1:A:144:ARG:O	1:A:147:VAL:HB	2.11	0.50
1:A:389:ILE:CG2	1:A:416:ILE:HA	2.40	0.50
1:B:1164:GLU:HG3	1:B:1225:ARG:NE	2.27	0.50
1:B:1342:TRP:CE3	1:B:1349:LEU:HD11	2.46	0.50
1:C:2153:ASN:O	1:C:2246:TYR:CE2	2.65	0.50
1:C:2396:GLY:HA2	1:C:2425:GLN:HA	1.94	0.50
1:C:2397:ARG:NH1	1:C:2429:THR:HG22	2.26	0.50
1:D:3276:PHE:C	1:D:3276:PHE:CD1	2.85	0.50
1:D:3327:MSE:O	1:D:3332:LEU:HB2	2.12	0.50
1:D:3507:LEU:O	1:D:3508:ALA:C	2.50	0.50
1:D:3313:GLY:HA3	3:D:3601:NAD:O5B	2.12	0.50
1:E:4302:ILE:HD13	1:E:4330:ASN:HB3	1.93	0.50
1:E:4351:VAL:HG13	1:E:4352:LYS:N	2.25	0.50
1:E:4492:LEU:O	1:E:4496:LYS:HG3	2.11	0.50
1:F:5166:ILE:HG21	1:F:5172:LEU:HD12	1.94	0.50
1:F:5184:LEU:HG	1:F:5198:CYS:HB3	1.93	0.50
1:G:6142:HIS:O	1:G:6145:SER:N	2.44	0.50
1:G:6155:VAL:HB	1:G:6246:TYR:CD2	2.46	0.50
1:G:6342:TRP:HZ3	1:G:6349:LEU:HD21	1.74	0.50
1:H:7172:LEU:O	1:H:7173:GLY:C	2.50	0.50
1:H:7176:GLY:O	1:H:7177:MSE:C	2.50	0.50
1:H:7266:LEU:HD22	1:H:7277:ASN:H	1.77	0.50
1:H:7412:GLU:CA	1:H:7440:ARG:NH1	2.74	0.50
1:A:295:GLN:HE22	1:A:305:HIS:CE1	2.28	0.50
1:A:295:GLN:O	1:A:298:ILE:N	2.45	0.50
1:A:279:ASP:HB3	1:A:314:GLU:OE1	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1122:GLN:O	1:B:1126:ILE:HG12	2.11	0.50
1:B:1221:LEU:HB3	1:B:1223:GLN:OE1	2.12	0.50
1:B:1240:LYS:O	1:B:1241:ALA:C	2.49	0.50
1:B:1317:LEU:CD1	1:B:1317:LEU:H	2.02	0.50
1:B:1324:VAL:HA	1:B:1327:MSE:HE3	1.93	0.50
1:E:4036:LYS:HB3	1:E:4039:ALA:HB3	1.94	0.50
1:E:4308:LEU:HD12	1:E:4342:TRP:O	2.12	0.50
1:F:5251:LEU:HD12	1:F:5252:ILE:H	1.73	0.50
1:F:5470:ILE:CD1	1:F:5498:LEU:HD22	2.42	0.50
1:F:5524:ILE:O	1:F:5528:ILE:HG13	2.11	0.50
1:H:7323:ILE:O	1:H:7325:MSE:N	2.45	0.50
1:H:7529:LYS:HD3	1:H:7532:GLU:OE1	2.11	0.50
1:A:152:GLU:CA	1:A:152:GLU:OE1	2.59	0.50
1:A:174:VAL:HG21	1:A:219:MSE:HG2	1.92	0.50
1:B:1371:GLU:HA	1:B:1371:GLU:OE1	2.10	0.50
1:B:1408:ALA:O	1:B:1411:ASN:O	2.28	0.50
1:B:1505:GLU:O	1:B:1509:GLN:HG2	2.11	0.50
1:C:2056:PRO:HB2	1:D:3221:LEU:HD13	1.94	0.50
1:D:3416:ILE:H	1:D:3416:ILE:HD13	1.77	0.50
1:D:3420:SER:HB3	1:D:3425:GLN:HB3	1.94	0.50
1:E:4031:ASN:OD1	1:E:4033:ARG:N	2.44	0.50
1:E:4238:PHE:O	1:E:4239:MSE:C	2.49	0.50
1:E:4380:ALA:HB1	1:E:4384:LEU:HD23	1.94	0.50
1:E:4453:LYS:CD	1:E:4457:GLY:HA2	2.41	0.50
1:E:4043:GLN:HG2	1:E:4566:LEU:HD11	1.93	0.50
1:F:5026:LYS:O	1:F:5029:MSE:N	2.44	0.50
1:G:6204:ASP:CG	1:G:6221:LEU:HB2	2.32	0.50
1:H:7324:VAL:HA	1:H:7327:MSE:HE3	1.93	0.50
1:A:184:LEU:HG	1:A:198:CYS:HB3	1.94	0.50
1:A:271:GLU:HA	1:A:485:HIS:CD2	2.46	0.50
1:A:480:LEU:O	1:A:542:ARG:HG3	2.11	0.50
1:B:1127:PHE:CD2	1:B:1127:PHE:C	2.85	0.50
1:C:2327:MSE:HE3	1:C:2337:ALA:HB1	1.94	0.50
1:C:2377:PHE:HZ	1:C:2389:ILE:HG12	1.77	0.50
1:D:3079:LEU:HG	1:D:3079:LEU:O	2.11	0.50
1:E:4264:ARG:CG	1:E:4265:PHE:N	2.75	0.50
1:E:4308:LEU:O	1:E:4389:ILE:HD12	2.11	0.50
1:E:4416:ILE:HD12	1:E:4441:CYS:HB2	1.94	0.50
1:F:5324:VAL:HG13	1:F:5337:ALA:HB3	1.94	0.50
1:G:6350:LEU:O	1:G:6366:THR:HA	2.12	0.50
1:G:6401:PRO:CA	1:G:6404:ILE:HD12	2.39	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:7194:ARG:CZ	1:H:7197:ARG:NH2	2.75	0.50
1:E:4142:HIS:CD2	1:H:7570:TYR:CE2	3.00	0.50
1:A:255:GLU:O	1:A:257:PHE:CD1	2.64	0.50
1:A:506:GLU:HG2	1:A:511:ARG:HD2	1.93	0.50
1:B:1487:SER:O	1:B:1490:VAL:HG23	2.12	0.50
1:B:1530:VAL:O	1:B:1533:TYR:HB3	2.12	0.50
1:B:1535:TYR:CE1	1:B:1546:PRO:HD2	2.46	0.50
1:C:2456:ASP:OD1	1:C:2458:ARG:HD3	2.12	0.50
1:D:3023:GLU:HG3	1:D:3024:LYS:N	2.27	0.50
1:E:4143:VAL:HG23	1:E:4237:GLU:OE2	2.11	0.50
1:F:5061:GLN:HA	1:F:5064:GLN:HE21	1.76	0.50
1:F:5288:LEU:O	1:F:5292:LEU:HG	2.12	0.50
1:F:5306:LYS:HB2	1:F:5306:LYS:NZ	2.27	0.50
1:F:5313:GLY:HA3	3:F:5601:NAD:O5B	2.12	0.50
1:G:6240:LYS:HA	1:G:6243:THR:OG1	2.12	0.50
1:G:6258:GLY:O	1:G:6260:HIS:N	2.45	0.50
1:H:7133:LEU:HB3	1:H:7201:VAL:HG22	1.93	0.50
1:H:7223:GLN:HG2	1:H:7224:LYS:O	2.11	0.50
1:A:124:GLY:O	1:B:1067:ARG:NE	2.44	0.49
1:A:128:ARG:HG3	1:B:1091:ARG:HH12	1.76	0.49
1:A:311:GLY:HA2	1:A:345:ASP:HA	1.94	0.49
1:A:429:THR:OG1	1:A:432:GLU:HG2	2.12	0.49
1:A:502:LEU:HD21	1:A:512:LEU:O	2.12	0.49
1:A:525:ASN:HA	1:A:528:ILE:HD12	1.94	0.49
1:B:1147:VAL:O	1:B:1245:ARG:NH1	2.45	0.49
1:B:1417:PHE:HA	1:B:1444:ALA:O	2.12	0.49
1:B:1503:THR:O	1:B:1507:LEU:N	2.44	0.49
1:C:2300:LYS:O	1:C:2305:HIS:NE2	2.45	0.49
1:C:2484:ARG:O	1:C:2485:HIS:ND1	2.45	0.49
1:A:572:TRP:CD1	1:D:3138:SER:O	2.64	0.49
1:D:3521:GLU:CA	1:D:3524:ILE:HD12	2.42	0.49
1:E:4352:LYS:CB	1:E:4368:SER:HA	2.42	0.49
1:E:4430:ALA:HA	1:E:4443:PHE:CE2	2.47	0.49
1:F:5104:ILE:O	1:F:5108:MSE:HE2	2.12	0.49
1:F:5194:ARG:NH2	1:F:5197:ARG:HE	2.02	0.49
1:F:5456:ASP:HB2	1:F:5458:ARG:CD	2.38	0.49
1:F:5572:TRP:NE1	1:G:6139:ASP:OD1	2.45	0.49
1:G:6340:LYS:C	1:G:6341:ILE:HG12	2.31	0.49
1:G:6396:GLY:O	1:G:6427:GLU:HA	2.11	0.49
1:G:6487:SER:O	1:G:6489:SER:N	2.45	0.49
1:G:6518:ASN:HB3	1:G:6521:GLU:OE2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:7099:ILE:O	1:H:7102:ASP:N	2.45	0.49
1:H:7172:LEU:O	1:H:7175:TYR:N	2.44	0.49
1:H:7179:ILE:O	1:H:7182:GLY:N	2.44	0.49
1:A:146:ILE:CD1	1:A:146:ILE:H	2.24	0.49
1:A:155:VAL:HB	1:A:246:TYR:CD2	2.47	0.49
1:A:388:THR:CG2	1:A:415:VAL:HB	2.42	0.49
1:B:1104:ILE:O	1:B:1108:MSE:HE2	2.11	0.49
1:B:1162:ASP:OD2	1:B:1164:GLU:OE1	2.30	0.49
1:B:1482:ASN:H	1:B:1482:ASN:HD22	1.60	0.49
1:B:1532:GLU:HG2	1:B:1549:LYS:HG3	1.94	0.49
1:C:2289:ALA:CB	1:C:2498:LEU:HD23	2.42	0.49
1:D:3491:PHE:O	1:D:3494:ALA:HB3	2.12	0.49
1:E:4059:GLU:OE2	1:E:4067:ARG:NH2	2.45	0.49
1:F:5142:HIS:O	1:F:5144:ARG:N	2.45	0.49
1:F:5528:ILE:HG21	1:F:5550:ALA:HA	1.94	0.49
1:G:6374:PRO:HG3	1:G:6380:ALA:CA	2.41	0.49
1:G:6306:LYS:O	1:G:6386:PRO:HB3	2.12	0.49
1:G:6452:VAL:O	1:G:6459:VAL:HA	2.13	0.49
1:H:7327:MSE:CE	1:H:7337:ALA:HB1	2.35	0.49
1:H:7396:GLY:HA2	1:H:7425:GLN:CA	2.42	0.49
1:A:396:GLY:O	1:A:398:LEU:HD13	2.12	0.49
1:A:458:ARG:HH11	1:A:458:ARG:HB2	1.76	0.49
1:A:67:ARG:O	1:A:71:ASN:ND2	2.44	0.49
1:B:1239:MSE:CE	1:B:1252:ILE:HD12	2.42	0.49
1:B:1258:GLY:O	1:B:1260:HIS:N	2.44	0.49
1:B:1298:ILE:CD1	1:B:1442:LEU:HD11	2.32	0.49
1:B:1474:VAL:O	1:B:1475:ALA:C	2.49	0.49
1:D:3375:ASP:OD2	1:D:3379:ASP:OD2	2.30	0.49
1:D:3487:SER:O	1:D:3490:VAL:HG23	2.12	0.49
1:E:4243:THR:HB	1:E:4248:ARG:NH1	2.27	0.49
1:F:5518:ASN:O	1:F:5522:VAL:HG23	2.12	0.49
1:H:7481:CYS:C	1:H:7483:THR:N	2.64	0.49
1:B:1358:ILE:N	1:B:1358:ILE:CD1	2.74	0.49
1:C:2258:GLY:O	1:C:2260:HIS:N	2.46	0.49
1:C:2352:LYS:CB	1:C:2368:SER:HA	2.43	0.49
1:C:2392:VAL:HG23	1:C:2419:LEU:HD23	1.95	0.49
1:C:2419:LEU:N	1:C:2419:LEU:CD2	2.67	0.49
1:D:3036:LYS:O	1:D:3039:ALA:HB3	2.13	0.49
1:D:3488:ASP:HA	1:D:3491:PHE:HD1	1.77	0.49
1:D:3528:ILE:HG21	1:D:3550:ALA:HA	1.95	0.49
1:E:4253:GLN:NE2	1:E:4255:GLU:HG2	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:4504:ASP:O	1:E:4507:LEU:N	2.44	0.49
1:E:4044:GLU:HG2	1:E:4566:LEU:HG	1.93	0.49
1:F:5188:THR:CG2	1:F:5195:PRO:HD3	2.42	0.49
1:F:5308:LEU:HD12	1:F:5342:TRP:O	2.11	0.49
1:F:5352:LYS:CG	1:F:5368:SER:HA	2.41	0.49
1:F:5419:LEU:HA	1:F:5446:GLY:H	1.76	0.49
1:G:6242:ILE:C	1:G:6244:ASP:N	2.64	0.49
1:H:7069:HIS:HE1	1:H:7102:ASP:OD2	1.95	0.49
1:A:86:MSE:HE2	1:A:86:MSE:N	2.27	0.49
1:C:2467:ASN:C	1:C:2469:TYR:H	2.15	0.49
1:D:3023:GLU:HG3	1:D:3024:LYS:H	1.78	0.49
1:E:4437:THR:C	1:E:4438:GLU:HG2	2.32	0.49
1:F:5251:LEU:C	1:F:5251:LEU:HD12	2.31	0.49
1:F:5303:SER:CA	1:F:5340:LYS:NZ	2.75	0.49
1:F:5376:THR:O	1:F:5379:ASP:HB2	2.12	0.49
1:G:6093:GLU:OE1	1:G:6195:PRO:HB2	2.12	0.49
1:H:7358:ILE:HG22	1:H:7362:GLN:HB3	1.93	0.49
1:H:7409:SER:O	1:H:7411:ASN:N	2.46	0.49
1:A:104:ILE:O	1:A:108:MSE:HE2	2.13	0.49
1:B:1057:LYS:HD2	1:B:1059:GLU:OE2	2.12	0.49
1:B:1152:GLU:HG3	1:B:1196:ASP:O	2.13	0.49
1:B:1376:THR:HG21	1:B:1378:GLU:HB3	1.94	0.49
1:C:2382:ASN:O	1:C:2383:ILE:C	2.51	0.49
1:C:2467:ASN:C	1:C:2469:TYR:N	2.64	0.49
1:C:2220:GLY:HA2	1:D:3056:PRO:HG2	1.94	0.49
1:D:3108:MSE:N	1:D:3109:PRO:HD2	2.28	0.49
1:D:3494:ALA:O	1:D:3497:ALA:N	2.46	0.49
1:E:4028:LEU:HD21	1:E:4048:LEU:HD12	1.93	0.49
1:E:4261:ASN:HA	1:E:4264:ARG:NE	2.27	0.49
1:G:6038:MSE:CE	1:G:6057:LYS:HB3	2.42	0.49
1:G:6389:ILE:CG2	1:G:6416:ILE:HG22	2.40	0.49
1:G:6476:LEU:O	1:G:6476:LEU:HD12	2.13	0.49
1:G:6549:LYS:HA	1:G:6552:TYR:HB3	1.94	0.49
1:H:7085:ILE:C	1:H:7087:GLY:H	2.15	0.49
1:H:7351:VAL:HG21	1:H:7370:PRO:HD3	1.94	0.49
1:H:7449:PHE:O	1:H:7462:PRO:HG2	2.12	0.49
1:A:413:ARG:HH21	1:A:440:ARG:C	2.15	0.49
1:B:1488:ASP:HA	1:B:1491:PHE:HD1	1.77	0.49
1:C:2048:LEU:N	1:C:2048:LEU:CD2	2.75	0.49
1:C:2504:ASP:O	1:C:2508:ALA:N	2.41	0.49
1:D:3288:LEU:HA	1:D:3291:LEU:HG	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:4412:GLU:O	1:E:4440:ARG:HB3	2.12	0.49
1:F:5565:LEU:HD23	1:F:5565:LEU:N	2.27	0.49
1:G:6466:ASN:ND2	1:G:6468:VAL:CG1	2.76	0.49
1:G:6494:ALA:O	1:G:6495:ALA:C	2.50	0.49
1:H:7253:GLN:HG3	1:H:7276:PHE:CZ	2.48	0.49
1:H:7412:GLU:CA	1:H:7440:ARG:HH11	2.24	0.49
1:A:136:SER:O	1:A:139:ASP:HB2	2.12	0.49
1:A:169:LEU:HD12	1:A:169:LEU:N	2.27	0.49
1:A:297:VAL:HG22	1:A:298:ILE:HD13	1.93	0.49
1:A:97:TYR:O	1:A:98:ARG:C	2.50	0.49
1:B:1079:LEU:O	1:B:1082:TYR:HB3	2.12	0.49
1:B:1093:GLU:OE1	1:B:1195:PRO:HB2	2.12	0.49
1:B:1428:CYS:SG	1:B:1429:THR:N	2.85	0.49
1:C:2400:THR:O	1:C:2404:ILE:HG13	2.13	0.49
1:C:2541:PHE:HD2	1:C:2541:PHE:N	2.10	0.49
1:D:3206:GLY:HA3	1:D:3223:GLN:HG2	1.94	0.49
1:D:3327:MSE:HE3	1:D:3337:ALA:CB	2.39	0.49
1:E:4095:LEU:HG	1:E:4099:ILE:HD12	1.95	0.49
1:E:4429:THR:HG23	1:E:4432:GLU:CD	2.33	0.49
1:F:5205:VAL:HG11	1:F:5231:TYR:HD1	1.78	0.49
1:F:5359:ASP:HB3	1:F:5362:GLN:OE1	2.12	0.49
1:G:6166:ILE:HG22	1:G:6166:ILE:O	2.12	0.49
1:H:7025:GLY:C	1:H:7027:PRO:HD2	2.33	0.49
1:H:7401:PRO:HA	1:H:7436:LEU:CD2	2.42	0.49
1:A:501:GLN:HA	1:A:501:GLN:HE21	1.75	0.49
1:B:1376:THR:H	1:B:1379:ASP:HB2	1.78	0.49
1:C:2057:LYS:HG3	1:D:3218:TYR:O	2.12	0.49
1:C:2384:LEU:O	1:C:2385:LYS:HB2	2.13	0.49
1:D:3123:TYR:HE1	1:D:3178:GLY:HA3	1.78	0.49
1:D:3297:VAL:HG22	1:D:3298:ILE:CD1	2.41	0.49
1:D:3349:LEU:HD23	1:D:3351:VAL:HB	1.95	0.49
1:D:3343:MSE:CE	1:D:3365:PHE:HB2	2.43	0.49
1:D:3439:GLY:HA3	1:D:3460:PHE:CE2	2.47	0.49
1:E:4332:LEU:CG	1:E:4336:GLU:OE2	2.61	0.49
1:E:4429:THR:HB	1:E:4449:PHE:CE2	2.48	0.49
1:E:4435:THR:OG1	1:E:4436:LEU:HD13	2.13	0.49
1:E:4540:ALA:O	1:E:4541:PHE:HD2	1.96	0.49
1:F:5298:ILE:HG22	4:F:8041:HOH:O	2.12	0.49
1:F:5399:PHE:HB2	1:F:5428:CYS:HB3	1.95	0.49
1:F:5429:THR:HG23	1:F:5432:GLU:HG2	1.94	0.49
1:G:6041:THR:CG2	1:G:6044:GLU:HG3	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:6351:VAL:HG13	1:G:6352:LYS:N	2.27	0.49
1:G:6419:LEU:HD13	1:G:6419:LEU:N	2.28	0.49
1:H:7481:CYS:SG	1:H:7534:LEU:CD1	3.00	0.49
1:A:566:LEU:HD22	1:A:567:PRO:HD2	1.93	0.49
1:B:1533:TYR:O	1:B:1534:LEU:C	2.51	0.49
1:C:2376:THR:HG22	1:C:2378:GLU:HB3	1.94	0.49
1:D:3123:TYR:CD2	1:D:3219:MSE:HE1	2.48	0.49
1:D:3287:ALA:O	1:D:3290:GLY:N	2.45	0.49
1:D:3319:ILE:O	1:D:3320:ALA:C	2.50	0.49
1:F:5144:ARG:HH12	1:F:5244:ASP:HB3	1.76	0.49
1:F:5333:SER:HG	1:F:5336:GLU:HG3	1.78	0.49
1:G:6310:LEU:HD21	1:G:6398:LEU:CB	2.42	0.49
1:G:6471:PHE:CD1	1:G:6472:PRO:HD3	2.47	0.49
1:H:7099:ILE:O	1:H:7102:ASP:HB2	2.12	0.49
1:H:7432:GLU:O	1:H:7436:LEU:HB2	2.12	0.49
1:H:7476:LEU:O	1:H:7476:LEU:HD12	2.12	0.49
1:A:270:ARG:CG	1:A:271:GLU:N	2.77	0.48
1:C:2160:VAL:HG11	1:C:2238:PHE:CZ	2.47	0.48
1:C:2244:ASP:N	1:C:2248:ARG:NH1	2.60	0.48
1:C:2324:VAL:HA	1:C:2327:MSE:CE	2.42	0.48
1:C:2502:LEU:HB3	1:C:2507:LEU:HD21	1.95	0.48
1:D:3150:TRP:HB3	1:D:3245:ARG:NH1	2.28	0.48
1:D:3275:THR:O	1:D:3486:ILE:HD11	2.13	0.48
1:E:4166:ILE:O	1:E:4167:LEU:C	2.52	0.48
1:E:4332:LEU:HD23	1:E:4337:ALA:N	2.27	0.48
1:E:4359:ASP:CG	1:E:4362:GLN:HG3	2.32	0.48
1:E:4363:GLU:CB	1:E:4364:PRO:CD	2.90	0.48
1:F:5302:ILE:N	1:F:5302:ILE:HD13	2.28	0.48
1:F:5374:PRO:HB3	1:F:5383:ILE:CD1	2.43	0.48
1:G:6413:ARG:NE	1:G:6440:ARG:O	2.45	0.48
1:H:7401:PRO:HB3	1:H:7436:LEU:HD21	1.95	0.48
1:A:191:ALA:HB3	1:A:193:ILE:HD12	1.94	0.48
1:A:397:ARG:HD2	1:A:397:ARG:H	1.78	0.48
1:C:2400:THR:CB	1:C:2401:PRO:HD2	2.43	0.48
1:C:2551:LYS:HG2	1:C:2555:GLU:CD	2.32	0.48
1:D:3359:ASP:O	1:D:3359:ASP:OD2	2.30	0.48
1:D:3479:ILE:O	1:D:3481:CYS:N	2.46	0.48
1:E:4025:GLY:O	1:E:4028:LEU:HB2	2.13	0.48
1:E:4188:THR:HG23	1:E:4193:ILE:O	2.13	0.48
1:E:4266:LEU:HD12	1:E:4266:LEU:C	2.33	0.48
1:E:4287:ALA:O	1:E:4290:GLY:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:6233:ASP:O	1:G:6237:GLU:N	2.43	0.48
1:G:6503:THR:O	1:G:6507:LEU:HD22	2.13	0.48
1:H:7453:LYS:HA	1:H:7458:ARG:O	2.13	0.48
1:H:7483:THR:OG1	1:H:7534:LEU:HD13	2.14	0.48
1:A:245:ARG:HG2	1:A:246:TYR:CE1	2.48	0.48
1:A:430:ALA:O	1:A:433:ALA:HB3	2.13	0.48
1:A:191:ALA:HB1	1:A:476:LEU:HD22	1.95	0.48
1:B:1147:VAL:HG21	1:B:1241:ALA:HB1	1.95	0.48
1:B:1290:GLY:O	1:B:1293:ALA:HB3	2.13	0.48
1:C:2425:GLN:O	1:C:2426:ALA:C	2.51	0.48
1:D:3294:ALA:O	1:D:3297:VAL:HG13	2.13	0.48
1:H:7556:ARG:HH11	1:H:7556:ARG:HG3	1.78	0.48
1:A:369:ALA:HB1	1:A:373:ILE:HD11	1.95	0.48
1:A:469:TYR:HB3	1:A:498:LEU:HD22	1.94	0.48
1:A:553:VAL:C	1:A:555:GLU:N	2.64	0.48
1:B:1099:ILE:O	1:B:1102:ASP:HB2	2.13	0.48
1:B:1264:ARG:HG3	1:B:1265:PHE:N	2.29	0.48
1:B:1431:GLU:C	1:B:1433:ALA:H	2.15	0.48
1:C:2300:LYS:NZ	1:C:2305:HIS:HA	2.28	0.48
1:C:2528:ILE:O	1:C:2531:THR:HG23	2.13	0.48
1:D:3028:LEU:HA	1:D:3028:LEU:HD12	1.66	0.48
1:D:3505:GLU:O	1:D:3508:ALA:HB3	2.14	0.48
1:G:6208:ASP:CG	1:G:6227:ARG:HH21	2.17	0.48
1:G:6307:ILE:CG2	1:G:6308:LEU:N	2.75	0.48
1:G:6402:ASP:HA	1:G:6405:ARG:CG	2.43	0.48
1:G:6541:PHE:N	1:G:6541:PHE:CD2	2.80	0.48
1:H:7309:PHE:CD2	1:H:7343:MSE:HG3	2.48	0.48
1:B:1043:GLN:HG3	1:B:1047:MSE:HE3	1.95	0.48
1:B:1471:PHE:CG	1:B:1472:PRO:HD3	2.48	0.48
1:C:2284:ALA:HA	1:C:2319:ILE:HG12	1.96	0.48
1:D:3261:ASN:O	1:D:3262:ALA:C	2.52	0.48
1:D:3300:LYS:HE3	1:D:3305:HIS:HD2	1.78	0.48
1:D:3370:PRO:O	1:D:3371:GLU:C	2.52	0.48
1:E:4300:LYS:HE2	1:E:4304:GLU:HB2	1.96	0.48
1:E:4320:ALA:HB1	1:E:4365:PHE:CE2	2.48	0.48
1:E:4363:GLU:HB3	1:E:4364:PRO:HD3	1.96	0.48
1:E:4470:ILE:HD11	1:E:4498:LEU:CD2	2.43	0.48
1:F:5559:ARG:HD3	1:F:5559:ARG:HA	1.49	0.48
1:G:6417:PHE:HB3	1:G:6419:LEU:HD11	1.95	0.48
1:H:7228:THR:OG1	1:H:7230:GLN:HG2	2.13	0.48
1:H:7287:ALA:O	1:H:7291:LEU:HG	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:7431:GLU:O	1:H:7433:ALA:N	2.45	0.48
1:A:23:GLU:HA	1:A:23:GLU:OE1	2.13	0.48
1:B:1559:ARG:HB3	1:B:1561:GLU:HG2	1.95	0.48
1:C:2454:LEU:HD12	1:C:2458:ARG:HB3	1.94	0.48
1:C:2471:PHE:CE1	1:C:2472:PRO:HG3	2.49	0.48
1:E:4104:ILE:HG23	1:E:4105:GLU:N	2.28	0.48
1:E:4152:GLU:HG2	1:E:4196:ASP:O	2.14	0.48
1:E:4212:LEU:C	1:E:4214:LYS:N	2.66	0.48
1:E:4456:ASP:OD2	1:E:4458:ARG:HD3	2.14	0.48
1:G:6104:ILE:CG2	1:G:6105:GLU:N	2.77	0.48
1:G:6227:ARG:HH11	1:G:6227:ARG:HG2	1.79	0.48
1:G:6406:ALA:O	1:G:6410:ILE:HG13	2.13	0.48
1:H:7085:ILE:HG23	1:H:7086:MSE:H	1.79	0.48
1:A:155:VAL:HB	1:A:246:TYR:CE2	2.49	0.48
1:A:376:THR:HB	1:A:379:ASP:OD2	2.14	0.48
1:A:421:ASN:N	3:A:601:NAD:O2D	2.46	0.48
1:A:437:THR:C	1:A:439:GLY:H	2.16	0.48
1:B:1036:LYS:O	1:B:1039:ALA:HB3	2.13	0.48
1:B:1194:ARG:CZ	1:B:1194:ARG:HB3	2.42	0.48
1:D:3150:TRP:HB3	1:D:3245:ARG:HH12	1.78	0.48
1:D:3261:ASN:CA	1:D:3264:ARG:HG2	2.43	0.48
1:D:3333:SER:HB3	1:D:3336:GLU:CD	2.34	0.48
1:D:3342:TRP:CH2	1:D:3367:HIS:HB2	2.49	0.48
1:D:3370:PRO:O	1:D:3373:ILE:HD12	2.13	0.48
1:D:3429:THR:OG1	1:D:3431:GLU:HB3	2.14	0.48
1:D:3530:VAL:O	1:D:3533:TYR:HB3	2.13	0.48
1:F:5078:PRO:HA	1:F:5081:LYS:HG3	1.96	0.48
1:F:5148:ASP:HA	1:F:5245:ARG:NH1	2.29	0.48
1:G:6033:ARG:HH11	1:G:6033:ARG:HG3	1.79	0.48
1:G:6234:LEU:HD12	1:G:6234:LEU:O	2.13	0.48
1:G:6350:LEU:CD1	1:G:6366:THR:HG23	2.42	0.48
1:G:6392:VAL:O	1:G:6393:ALA:HB2	2.14	0.48
1:G:6396:GLY:HA2	1:G:6425:GLN:HA	1.96	0.48
1:G:6478:VAL:HG12	1:G:6479:ILE:CD1	2.37	0.48
1:H:7505:GLU:O	1:H:7508:ALA:HB3	2.13	0.48
1:A:243:THR:C	1:A:248:ARG:HH11	2.16	0.48
1:A:267:ARG:HG3	1:A:267:ARG:NH1	2.24	0.48
1:A:310:LEU:HD22	1:A:399:PHE:CE2	2.48	0.48
1:A:479:ILE:HG22	1:A:480:LEU:N	2.27	0.48
1:B:1208:ASP:OD1	1:B:1224:LYS:HG3	2.13	0.48
1:B:1271:GLU:O	1:B:1485:HIS:NE2	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2257:PHE:HB3	1:C:2262:ALA:HB2	1.96	0.48
1:C:2292:LEU:O	1:C:2294:ALA:N	2.47	0.48
1:C:2470:ILE:HD11	1:C:2498:LEU:HD22	1.95	0.48
1:C:2524:ILE:O	1:C:2527:ALA:HB3	2.14	0.48
1:D:3302:ILE:O	1:D:3303:SER:C	2.52	0.48
1:D:3491:PHE:O	1:D:3494:ALA:N	2.46	0.48
1:E:4281:GLN:HB3	1:E:4491:PHE:CZ	2.49	0.48
1:E:4392:VAL:CG2	1:E:4419:LEU:HD23	2.44	0.48
1:F:5402:ASP:HA	1:F:5405:ARG:CG	2.43	0.48
1:G:6209:ASN:HB3	1:G:6212:LEU:HD12	1.95	0.48
1:G:6238:PHE:CE1	1:G:6242:ILE:HG13	2.49	0.48
1:G:6302:ILE:O	1:G:6303:SER:C	2.52	0.48
1:G:6354:ARG:HE	1:G:6356:ALA:CB	2.18	0.48
1:A:145:SER:OG	1:A:146:ILE:HD12	2.13	0.48
1:B:1341:ILE:O	1:B:1367:HIS:NE2	2.47	0.48
1:B:1390:ILE:HG23	1:B:1419:LEU:CD2	2.44	0.48
1:B:1453:LYS:CG	1:B:1459:VAL:HG13	2.43	0.48
1:B:1527:ALA:O	1:B:1531:THR:CG2	2.58	0.48
1:C:2081:LYS:O	1:C:2085:ILE:HG22	2.14	0.48
1:C:2090:GLU:HG3	1:C:2131:LYS:HD3	1.94	0.48
1:C:2454:LEU:O	1:C:2456:ASP:N	2.47	0.48
1:D:3218:TYR:CE2	4:D:8046:HOH:O	2.36	0.48
1:D:3306:LYS:HD2	1:D:3384:LEU:O	2.14	0.48
1:D:3506:GLU:HB3	1:D:3511:ARG:HD2	1.96	0.48
1:E:4043:GLN:HG2	1:E:4566:LEU:CD1	2.44	0.48
1:G:6143:VAL:HG21	1:G:6237:GLU:HG2	1.96	0.48
1:G:6342:TRP:CE2	1:G:6384:LEU:HD11	2.48	0.48
1:H:7060:THR:HG23	1:H:7063:ILE:CD1	2.35	0.48
1:H:7278:ASP:C	1:H:7280:ILE:N	2.66	0.48
1:A:166:ILE:O	1:A:167:LEU:C	2.52	0.48
1:A:385:LYS:HG3	1:A:410:ILE:HG21	1.95	0.48
1:A:494:ALA:O	1:A:497:ALA:HB3	2.14	0.48
1:B:1038:MSE:HB3	1:B:1057:LYS:O	2.14	0.48
1:B:1375:ASP:OD2	1:B:1379:ASP:OD2	2.32	0.48
1:B:1378:GLU:O	1:B:1381:VAL:HB	2.13	0.48
1:B:1392:VAL:HG12	4:B:8059:HOH:O	2.12	0.48
1:C:2268:LYS:HE2	1:C:2269:TYR:CZ	2.49	0.48
1:C:2270:ARG:NH2	1:C:2486:ILE:O	2.45	0.48
1:D:3041:THR:HG23	1:D:3044:GLU:CD	2.34	0.48
1:D:3082:TYR:HA	1:D:3110:ILE:CG2	2.44	0.48
1:D:3104:ILE:O	1:D:3108:MSE:HE2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3194:ARG:HB2	1:D:3197:ARG:HG3	1.94	0.48
1:D:3374:PRO:HD3	1:D:3383:ILE:HG21	1.95	0.48
1:E:4105:GLU:HA	1:E:4108:MSE:CE	2.44	0.48
1:E:4206:GLY:HA3	1:E:4223:GLN:NE2	2.27	0.48
1:E:4332:LEU:CD2	1:E:4337:ALA:HA	2.44	0.48
1:E:4398:LEU:HD12	1:E:4398:LEU:N	2.29	0.48
1:F:5144:ARG:HH12	1:F:5244:ASP:CB	2.27	0.48
1:G:6283:THR:O	1:G:6284:ALA:C	2.51	0.48
1:G:6314:GLU:HG2	3:G:6601:NAD:O1N	2.14	0.48
1:H:7096:PHE:HA	1:H:7099:ILE:HD12	1.95	0.48
1:H:7484:ARG:C	1:H:7485:HIS:ND1	2.67	0.48
1:H:7559:ARG:HA	1:H:7559:ARG:HD3	1.60	0.48
1:A:445:SER:O	1:A:464:GLN:HA	2.13	0.47
1:B:1177:MSE:CE	1:B:1180:PRO:HB2	2.44	0.47
1:B:1177:MSE:O	1:B:1177:MSE:HE3	2.13	0.47
1:B:1272:LYS:O	1:B:1273:TYR:CD2	2.67	0.47
1:B:1300:LYS:HE2	1:B:1304:GLU:OE2	2.14	0.47
1:B:1300:LYS:HZ1	1:B:1305:HIS:HA	1.78	0.47
1:B:1349:LEU:HG	1:B:1350:LEU:N	2.29	0.47
1:C:2306:LYS:O	1:C:2387:SER:N	2.47	0.47
1:D:3194:ARG:CZ	1:D:3196:ASP:OD2	2.62	0.47
1:D:3290:GLY:O	1:D:3291:LEU:C	2.51	0.47
1:D:3359:ASP:OD2	1:D:3359:ASP:C	2.52	0.47
1:D:3351:VAL:HG22	1:D:3367:HIS:O	2.14	0.47
1:E:4425:GLN:HE21	1:E:4425:GLN:N	2.13	0.47
1:F:5382:ASN:O	1:F:5385:LYS:HD3	2.14	0.47
1:G:6041:THR:HG23	1:G:6044:GLU:CD	2.34	0.47
1:G:6357:LYS:C	1:G:6358:ILE:HG13	2.34	0.47
1:G:6389:ILE:HD12	1:G:6389:ILE:HA	1.68	0.47
1:G:6429:THR:HG23	1:G:6432:GLU:OE1	2.14	0.47
1:G:6559:ARG:HD3	1:G:6559:ARG:HA	1.62	0.47
1:H:7043:GLN:HG2	1:H:7566:LEU:CD1	2.39	0.47
1:H:7425:GLN:N	1:H:7425:GLN:NE2	2.62	0.47
1:A:266:LEU:O	1:A:270:ARG:HB3	2.15	0.47
1:A:524:ILE:HG22	1:A:525:ASN:N	2.29	0.47
1:B:1391:GLY:N	1:B:1417:PHE:O	2.41	0.47
1:B:1528:ILE:O	1:B:1532:GLU:HG3	2.14	0.47
1:C:2223:GLN:HG2	1:C:2224:LYS:O	2.14	0.47
1:D:3147:VAL:O	1:D:3245:ARG:NH1	2.47	0.47
1:D:3288:LEU:CD2	1:D:3292:LEU:HG	2.44	0.47
1:D:3414:PRO:HD2	1:D:3440:ARG:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:5135:ILE:O	1:F:5203:ILE:HA	2.13	0.47
1:F:5266:LEU:HD12	1:F:5266:LEU:O	2.14	0.47
1:F:5535:TYR:CD2	1:F:5540:ALA:HB3	2.50	0.47
1:F:5542:ARG:C	1:F:5542:ARG:HD3	2.34	0.47
1:F:5094:LYS:NZ	1:F:5559:ARG:O	2.38	0.47
1:G:6317:LEU:N	1:G:6317:LEU:HD12	2.08	0.47
1:G:6431:GLU:O	1:G:6433:ALA:N	2.42	0.47
1:H:7417:PHE:HA	1:H:7444:ALA:O	2.14	0.47
1:A:143:VAL:O	1:A:146:ILE:HB	2.14	0.47
1:A:148:ASP:HA	1:A:245:ARG:NH1	2.28	0.47
1:A:308:LEU:HD13	1:A:342:TRP:HB2	1.96	0.47
1:B:1505:GLU:CD	1:B:1505:GLU:N	2.66	0.47
1:D:3186:LEU:HA	1:D:3189:ALA:HB3	1.96	0.47
1:D:3210:ILE:CB	1:D:3214:LYS:HZ2	2.25	0.47
1:E:4031:ASN:OD1	1:E:4033:ARG:HB2	2.14	0.47
1:E:4291:LEU:HD23	1:E:4417:PHE:CE2	2.50	0.47
1:E:4389:ILE:HA	1:E:4389:ILE:HD12	1.69	0.47
1:F:5537:ASN:O	1:F:5538:LYS:C	2.52	0.47
1:G:6135:ILE:HD13	1:G:6143:VAL:HG13	1.96	0.47
1:G:6528:ILE:HD11	1:G:6554:LYS:HD2	1.94	0.47
1:H:7123:TYR:O	1:H:7175:TYR:CZ	2.67	0.47
1:H:7399:PHE:HA	1:H:7403:VAL:HG11	1.96	0.47
1:A:261:ASN:HA	1:A:264:ARG:HE	1.79	0.47
1:B:1227:ARG:NH1	1:B:1227:ARG:HG2	2.12	0.47
1:C:2416:ILE:N	1:C:2416:ILE:CD1	2.78	0.47
1:C:2454:LEU:HD12	1:C:2458:ARG:CB	2.44	0.47
1:D:3094:LYS:HG2	1:D:3562:TYR:HD2	1.79	0.47
1:D:3142:HIS:O	1:D:3143:VAL:C	2.52	0.47
1:D:3116:VAL:CG2	1:D:3179:ILE:HD13	2.44	0.47
1:D:3281:GLN:HG2	1:D:3491:PHE:CE1	2.50	0.47
1:D:3286:VAL:O	1:D:3289:ALA:HB3	2.13	0.47
1:E:4059:GLU:CD	1:E:4067:ARG:HH22	2.17	0.47
1:E:4261:ASN:HD22	1:E:4261:ASN:N	2.03	0.47
1:E:4506:GLU:O	1:E:4511:ARG:HG3	2.14	0.47
1:F:5127:PHE:O	1:F:5128:ARG:HD3	2.13	0.47
1:G:6306:LYS:O	1:G:6386:PRO:CB	2.63	0.47
1:G:6508:ALA:C	1:G:6510:GLY:H	2.18	0.47
1:G:6525:ASN:O	1:G:6526:ILE:C	2.52	0.47
1:H:7351:VAL:CG1	1:H:7369:ALA:HB2	2.44	0.47
1:A:143:VAL:HG11	1:A:238:PHE:HA	1.95	0.47
1:A:239:MSE:HE2	1:A:269:TYR:CD1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:GLY:O	1:B:1133:LEU:HD12	2.14	0.47
1:B:1137:ILE:HB	1:B:1205:VAL:HG12	1.95	0.47
1:B:1344:PHE:HA	1:B:1349:LEU:HA	1.97	0.47
1:B:1407:MSE:SE	1:B:1411:ASN:HD21	2.48	0.47
1:C:2429:THR:HA	1:C:2449:PHE:CZ	2.50	0.47
1:D:3068:PHE:CZ	1:D:3085:ILE:HD12	2.49	0.47
1:D:3243:THR:HB	1:D:3248:ARG:HH11	1.79	0.47
1:D:3304:GLU:H	1:D:3304:GLU:HG3	1.34	0.47
1:E:4075:MSE:HG3	1:E:4080:GLU:CD	2.35	0.47
1:F:5081:LYS:O	1:F:5082:TYR:C	2.52	0.47
1:F:5559:ARG:NH1	1:F:5559:ARG:CG	2.76	0.47
1:G:6122:GLN:HA	1:G:6122:GLN:NE2	2.29	0.47
1:G:6333:SER:OG	1:G:6335:GLN:HB3	2.14	0.47
1:G:6416:ILE:CD1	1:G:6441:CYS:HB2	2.44	0.47
1:H:7136:SER:O	1:H:7139:ASP:HB2	2.13	0.47
1:H:7166:ILE:O	1:H:7169:LEU:HB2	2.14	0.47
1:H:7297:VAL:HG22	1:H:7298:ILE:HD13	1.96	0.47
1:H:7374:PRO:HB3	1:H:7380:ALA:N	2.30	0.47
1:H:7459:VAL:O	1:H:7460:PHE:HD1	1.96	0.47
1:H:7468:VAL:HA	1:H:7471:PHE:CE2	2.49	0.47
1:H:7527:ALA:O	1:H:7531:THR:HG23	2.14	0.47
1:A:276:PHE:HB2	1:A:281:GLN:HE22	1.74	0.47
1:B:1050:LEU:O	1:B:1053:LEU:HB2	2.15	0.47
1:B:1389:ILE:HG23	1:B:1399:PHE:CE1	2.50	0.47
1:B:1273:TYR:O	1:B:1485:HIS:HD2	1.98	0.47
1:C:2300:LYS:HZ3	1:C:2305:HIS:HA	1.79	0.47
1:C:2328:VAL:HG22	1:C:2332:LEU:O	2.13	0.47
1:C:2503:THR:HG23	1:C:2506:GLU:OE1	2.14	0.47
1:D:3046:GLN:HG2	1:D:3051:GLN:HG3	1.97	0.47
1:D:3088:ILE:HD12	1:D:3091:ARG:NH1	2.30	0.47
1:D:3123:TYR:C	1:D:3125:HIS:H	2.18	0.47
1:D:3255:GLU:O	1:D:3256:ASP:C	2.53	0.47
1:E:4300:LYS:CE	1:E:4304:GLU:HB2	2.44	0.47
1:E:4388:THR:HG23	1:E:4415:VAL:CG1	2.45	0.47
1:G:6278:ASP:C	1:G:6280:ILE:H	2.17	0.47
1:H:7412:GLU:C	1:H:7440:ARG:HH11	2.17	0.47
1:H:7467:ASN:C	1:H:7469:TYR:N	2.67	0.47
1:B:1302:ILE:O	1:B:1304:GLU:N	2.47	0.47
1:B:1381:VAL:HG13	1:B:1407:MSE:HE2	1.96	0.47
1:B:1411:ASN:O	1:B:1440:ARG:NH1	2.48	0.47
1:B:1474:VAL:O	1:B:1477:ALA:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1561:GLU:H	1:B:1561:GLU:HG2	1.50	0.47
1:C:2150:TRP:NE1	1:C:2152:GLU:HB2	2.30	0.47
1:C:2329:GLU:O	1:C:2329:GLU:HG3	2.13	0.47
1:C:2357:LYS:C	1:C:2358:ILE:HG13	2.35	0.47
1:C:2559:ARG:CG	1:C:2561:GLU:HG2	2.44	0.47
1:C:2467:ASN:OD1	3:C:2601:NAD:N7N	2.47	0.47
1:D:3284:ALA:O	1:D:3286:VAL:N	2.48	0.47
1:D:3303:SER:O	1:D:3340:LYS:HE2	2.13	0.47
1:D:3333:SER:OG	1:D:3335:GLN:HB3	2.14	0.47
1:D:3504:ASP:O	1:D:3507:LEU:HB2	2.14	0.47
1:D:3538:LYS:HA	1:D:3538:LYS:HD3	1.41	0.47
1:D:3561:GLU:H	1:D:3561:GLU:HG2	1.38	0.47
1:E:4187:TYR:O	1:E:4191:ALA:HB3	2.14	0.47
1:E:4147:VAL:O	1:E:4245:ARG:NH1	2.48	0.47
1:E:4379:ASP:O	1:E:4380:ALA:C	2.53	0.47
1:E:4385:LYS:HB2	1:E:4385:LYS:HE2	1.45	0.47
1:F:5352:LYS:HG2	1:F:5368:SER:N	2.28	0.47
1:F:5470:ILE:HG22	1:F:5474:VAL:CG2	2.43	0.47
1:G:6323:ILE:HG22	1:G:6327:MSE:CE	2.27	0.47
1:G:6488:ASP:HA	1:G:6491:PHE:CD1	2.41	0.47
1:H:7230:GLN:HG2	1:H:7230:GLN:H	1.55	0.47
1:A:152:GLU:N	1:A:152:GLU:OE1	2.48	0.47
1:A:212:LEU:O	1:A:215:ASP:N	2.36	0.47
1:A:259:ASN:HD22	1:A:259:ASN:N	2.11	0.47
1:A:313:GLY:O	1:A:314:GLU:C	2.53	0.47
1:A:376:THR:CG2	1:A:378:GLU:HB3	2.45	0.47
1:A:381:VAL:HG13	1:A:407:MSE:CE	2.44	0.47
1:B:1045:ARG:NH2	1:B:1058:ILE:HD13	2.29	0.47
1:C:2028:LEU:CD2	1:C:2048:LEU:HD12	2.45	0.47
1:C:2075:MSE:HG3	1:C:2080:GLU:OE1	2.15	0.47
1:C:2341:ILE:O	1:C:2367:HIS:NE2	2.39	0.47
1:D:3343:MSE:HE2	1:D:3365:PHE:HB2	1.96	0.47
1:D:3421:ASN:HA	1:D:3422:PRO:C	2.32	0.47
1:F:5025:GLY:O	1:F:5050:LEU:HD21	2.15	0.47
1:G:6165:ARG:CZ	1:G:6259:ASN:HD21	2.27	0.47
1:G:6210:ILE:C	1:G:6214:LYS:HD2	2.34	0.47
1:G:6384:LEU:HB3	1:G:6386:PRO:HD3	1.97	0.47
1:G:6402:ASP:CA	1:G:6405:ARG:HG2	2.44	0.47
1:G:6416:ILE:HD11	1:G:6441:CYS:SG	2.55	0.47
1:G:6492:LEU:O	1:G:6495:ALA:N	2.47	0.47
1:G:6498:LEU:HA	1:G:6526:ILE:HD11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:7112:TYR:CD2	1:H:7113:THR:HG23	2.50	0.47
1:H:7243:THR:C	1:H:7248:ARG:NH1	2.66	0.47
1:H:7373:ILE:HG22	1:H:7373:ILE:O	2.14	0.47
1:H:7390:ILE:HG23	1:H:7417:PHE:CB	2.42	0.47
1:H:7434:TYR:CD2	1:H:7441:CYS:SG	3.08	0.47
1:H:7043:GLN:CG	1:H:7566:LEU:HD11	2.39	0.47
1:A:182:GLY:O	1:A:185:CYS:HB2	2.15	0.47
1:A:397:ARG:HH11	1:A:397:ARG:CG	2.27	0.47
1:A:425:GLN:N	1:A:425:GLN:NE2	2.62	0.47
1:B:1108:MSE:HB3	1:B:1109:PRO:CD	2.44	0.47
1:B:1123:TYR:CD2	1:B:1219:MSE:HE1	2.50	0.47
1:B:1253:GLN:HG3	1:B:1276:PHE:CE2	2.49	0.47
1:B:1300:LYS:O	1:B:1304:GLU:OE2	2.33	0.47
1:B:1347:TYR:CD1	1:B:1356:ALA:HB1	2.50	0.47
1:B:1451:PRO:HA	1:B:1461:THR:HA	1.97	0.47
1:B:1470:ILE:C	1:B:1472:PRO:CD	2.83	0.47
1:C:2060:THR:OG1	1:C:2063:ILE:HG13	2.14	0.47
1:C:2377:PHE:CE1	1:C:2389:ILE:HD11	2.50	0.47
1:C:2386:PRO:HG2	1:C:2407:MSE:SE	2.65	0.47
1:C:2395:ALA:O	1:C:2398:LEU:HD11	2.15	0.47
1:D:3103:ASP:HB3	1:D:3107:LEU:CD2	2.43	0.47
1:D:3234:LEU:O	1:D:3238:PHE:HB3	2.14	0.47
1:D:3165:ARG:HB2	1:D:3257:PHE:O	2.14	0.47
1:D:3288:LEU:HG	1:D:3292:LEU:HD23	1.96	0.47
1:D:3342:TRP:CE2	1:D:3367:HIS:CD2	3.03	0.47
1:G:6535:TYR:CZ	1:G:6545:GLU:HA	2.49	0.47
1:H:7243:THR:HG21	1:H:7273:TYR:CD2	2.50	0.47
1:A:180:PRO:HB2	1:A:200:PRO:HB2	1.97	0.47
1:A:349:LEU:HD21	1:A:351:VAL:CG2	2.45	0.47
1:A:389:ILE:CG2	1:A:416:ILE:HG22	2.45	0.47
1:A:512:LEU:CD1	1:A:512:LEU:H	2.25	0.47
1:B:1075:MSE:HG3	1:B:1080:GLU:CD	2.35	0.47
1:B:1273:TYR:O	1:B:1485:HIS:CD2	2.68	0.47
1:B:1521:GLU:O	1:B:1522:VAL:C	2.51	0.47
1:C:2188:THR:HG21	1:C:2195:PRO:HG3	1.96	0.47
1:C:2260:HIS:C	1:C:2260:HIS:ND1	2.67	0.47
1:C:2291:LEU:O	1:C:2294:ALA:HB3	2.15	0.47
1:C:2310:LEU:HG	1:C:2310:LEU:O	2.14	0.47
1:C:2400:THR:HB	1:C:2401:PRO:HD2	1.95	0.47
1:D:3273:TYR:HB2	1:D:3275:THR:HG22	1.96	0.47
1:D:3300:LYS:NZ	1:D:3305:HIS:N	2.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3471:PHE:CG	1:D:3472:PRO:CD	2.95	0.47
1:D:3482:ASN:ND2	1:D:3542:ARG:HB2	2.30	0.47
1:E:4026:LYS:C	1:E:4028:LEU:N	2.68	0.47
1:E:4207:THR:OG1	1:E:4208:ASP:N	2.48	0.47
1:E:4303:SER:HA	1:E:4340:LYS:HZ3	1.80	0.47
1:E:4405:ARG:CG	1:E:4406:ALA:N	2.77	0.47
1:E:4405:ARG:HG3	1:E:4406:ALA:N	2.30	0.47
1:G:6160:VAL:HG11	1:G:6238:PHE:CZ	2.50	0.47
1:H:7076:THR:HB	1:H:7077:SER:H	1.55	0.47
1:B:1174:VAL:HG23	1:B:1219:MSE:CE	2.45	0.47
1:B:1312:ALA:CB	1:B:1362:GLN:HE21	2.27	0.47
1:B:1552:TYR:CE1	1:B:1556:ARG:CZ	2.98	0.47
1:C:2072:LEU:O	1:C:2075:MSE:HB2	2.14	0.47
1:C:2176:GLY:C	1:C:2178:GLY:N	2.69	0.47
1:C:2313:GLY:O	1:C:2316:ALA:N	2.43	0.47
1:C:2317:LEU:H	1:C:2317:LEU:CD1	2.10	0.47
1:D:3416:ILE:HD13	1:D:3442:LEU:O	2.15	0.47
1:E:4077:SER:O	1:E:4080:GLU:HB3	2.15	0.47
1:E:4085:ILE:HG23	1:E:4086:MSE:N	2.30	0.47
1:E:4108:MSE:HE2	1:E:4108:MSE:HB2	1.74	0.47
1:E:4196:ASP:N	1:E:4196:ASP:OD1	2.48	0.47
1:E:4208:ASP:OD1	1:E:4224:LYS:HD2	2.15	0.47
1:G:6128:ARG:HH11	1:G:6128:ARG:CG	2.26	0.47
1:G:6302:ILE:HD12	1:G:6302:ILE:H	1.80	0.47
1:G:6321:ASN:O	1:G:6322:LEU:C	2.52	0.47
1:G:6428:CYS:SG	1:G:6429:THR:N	2.88	0.47
1:G:6541:PHE:N	1:G:6541:PHE:HD2	2.13	0.47
1:H:7255:GLU:O	1:H:7256:ASP:C	2.52	0.47
1:H:7377:PHE:O	1:H:7378:GLU:C	2.53	0.47
1:A:142:HIS:O	1:A:143:VAL:C	2.53	0.46
1:A:372:SER:OG	1:A:383:ILE:HD13	2.15	0.46
1:B:1068:PHE:CZ	1:B:1085:ILE:HD12	2.50	0.46
1:B:1210:ILE:O	1:B:1214:LYS:HG3	2.15	0.46
1:B:1232:ASP:O	1:B:1235:ILE:HG12	2.15	0.46
1:B:1281:GLN:HG2	1:B:1491:PHE:CE1	2.50	0.46
1:B:1369:ALA:HB1	1:B:1373:ILE:HD11	1.96	0.46
1:C:2253:GLN:NE2	1:C:2255:GLU:HG2	2.30	0.46
1:E:4060:THR:O	1:E:4064:GLN:HG2	2.15	0.46
1:E:4310:LEU:HG	1:E:4310:LEU:O	2.15	0.46
1:E:4402:ASP:CA	1:E:4405:ARG:HG2	2.42	0.46
1:E:4494:ALA:O	1:E:4497:ALA:HB3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:4501:GLN:HB3	1:E:4514:PRO:HG3	1.97	0.46
1:F:5071:ASN:O	1:F:5075:MSE:CE	2.63	0.46
1:F:5108:MSE:N	1:F:5109:PRO:HD2	2.29	0.46
1:F:5228:THR:OG1	1:F:5229:GLN:N	2.47	0.46
1:F:5358:ILE:HG21	1:F:5366:THR:OG1	2.15	0.46
1:F:5378:GLU:HA	1:F:5381:VAL:CG2	2.45	0.46
1:G:6209:ASN:C	1:G:6213:LEU:HD12	2.35	0.46
1:G:6287:ALA:O	1:G:6290:GLY:N	2.44	0.46
1:G:6394:GLY:HA2	1:G:6425:GLN:HG3	1.97	0.46
1:H:7289:ALA:HA	1:H:7499:THR:OG1	2.15	0.46
1:A:245:ARG:HG2	1:A:246:TYR:CD1	2.50	0.46
1:A:281:GLN:HG2	1:A:491:PHE:CE1	2.50	0.46
1:A:341:ILE:HB	1:A:365:PHE:CD2	2.50	0.46
1:A:82:TYR:CD2	1:A:82:TYR:C	2.89	0.46
1:B:1155:VAL:HB	1:B:1246:TYR:CD2	2.50	0.46
1:B:1512:LEU:HD12	1:B:1512:LEU:H	1.81	0.46
1:B:1556:ARG:HG3	1:B:1556:ARG:HH11	1.79	0.46
1:C:2140:ARG:NH1	1:C:2230:GLN:HG2	2.30	0.46
1:C:2150:TRP:CD1	1:C:2152:GLU:HB2	2.50	0.46
1:C:2278:ASP:O	1:C:2280:ILE:N	2.49	0.46
1:C:2308:LEU:HB3	1:C:2389:ILE:HD12	1.95	0.46
1:C:2374:PRO:CB	1:C:2379:ASP:HB3	2.46	0.46
1:C:2503:THR:O	1:C:2507:LEU:HD23	2.15	0.46
1:C:2520:GLN:O	1:C:2523:SER:N	2.47	0.46
1:D:3104:ILE:HG23	1:D:3105:GLU:N	2.30	0.46
1:D:3123:TYR:CE1	1:D:3178:GLY:HA3	2.50	0.46
1:D:3156:LYS:HD3	1:D:3479:ILE:HG23	1.96	0.46
1:D:3168:GLY:C	1:D:3169:LEU:HD12	2.35	0.46
1:D:3402:ASP:CA	1:D:3405:ARG:HG2	2.45	0.46
1:E:4438:GLU:O	1:E:4458:ARG:NH1	2.49	0.46
1:E:4467:ASN:OD1	3:E:4601:NAD:N7N	2.48	0.46
1:F:5231:TYR:O	1:F:5235:ILE:HG12	2.16	0.46
1:F:5308:LEU:HD12	1:F:5309:PHE:H	1.80	0.46
1:G:6338:GLN:HA	1:G:6341:ILE:HG13	1.97	0.46
1:G:6397:ARG:CZ	1:G:6429:THR:HG22	2.45	0.46
1:H:7071:ASN:O	1:H:7075:MSE:HE3	2.15	0.46
1:A:103:ASP:HB3	1:A:107:LEU:CD2	2.35	0.46
1:A:139:ASP:O	1:A:140:ARG:C	2.51	0.46
1:A:41:THR:HG23	1:A:44:GLU:OE2	2.15	0.46
1:A:476:LEU:CD1	1:A:480:LEU:HD11	2.45	0.46
1:A:38:MSE:SE	1:B:1219:MSE:HB3	2.65	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1400:THR:HB	1:B:1401:PRO:HD2	1.98	0.46
1:B:1466:ASN:HB3	1:B:1468:VAL:CG1	2.32	0.46
1:C:2197:ARG:NH1	1:C:2197:ARG:CG	2.65	0.46
1:C:2183:LYS:NZ	1:C:2255:GLU:OE2	2.29	0.46
1:D:3424:ALA:C	1:D:3425:GLN:NE2	2.68	0.46
1:D:3432:GLU:O	1:D:3433:ALA:C	2.53	0.46
1:D:3454:LEU:HD12	1:D:3458:ARG:HB2	1.97	0.46
1:D:3548:ASP:OD1	1:D:3550:ALA:HB3	2.15	0.46
1:E:4492:LEU:O	1:E:4495:ALA:HB3	2.15	0.46
1:E:4553:VAL:O	1:E:4555:GLU:N	2.48	0.46
1:F:5159:VAL:HG21	1:F:5184:LEU:HD13	1.96	0.46
1:G:6060:THR:O	1:G:6061:GLN:C	2.53	0.46
1:G:6075:MSE:HG3	1:G:6080:GLU:HG2	1.95	0.46
1:G:6086:MSE:HE3	1:G:6086:MSE:CA	2.46	0.46
1:G:6086:MSE:CE	1:G:6096:PHE:HE1	2.29	0.46
1:G:6188:THR:HG23	1:G:6195:PRO:HD3	1.97	0.46
1:G:6402:ASP:HA	1:G:6405:ARG:CD	2.45	0.46
1:G:6413:ARG:HA	1:G:6413:ARG:HE	1.79	0.46
1:G:6430:ALA:HA	1:G:6443:PHE:CE2	2.49	0.46
1:H:7123:TYR:C	1:H:7125:HIS:H	2.19	0.46
1:H:7306:LYS:NZ	1:H:7384:LEU:O	2.49	0.46
1:H:7308:LEU:HB3	1:H:7389:ILE:HD13	1.97	0.46
1:H:7521:GLU:O	1:H:7522:VAL:C	2.53	0.46
1:H:7543:TYR:HB2	1:H:7544:PRO:HA	1.96	0.46
1:A:277:ASN:N	1:A:281:GLN:OE1	2.41	0.46
1:A:431:GLU:O	1:A:433:ALA:N	2.48	0.46
1:A:454:LEU:HD12	1:A:458:ARG:O	2.16	0.46
1:A:271:GLU:O	1:A:485:HIS:NE2	2.48	0.46
1:B:1171:ASP:OD2	1:B:1225:ARG:NE	2.49	0.46
1:B:1363:GLU:CB	1:B:1364:PRO:HD3	2.46	0.46
1:B:1376:THR:O	1:B:1379:ASP:HB2	2.16	0.46
1:C:2552:TYR:O	1:C:2555:GLU:HB2	2.14	0.46
1:A:42:LEU:CD2	1:C:2572:TRP:HB2	2.45	0.46
1:D:3419:LEU:HA	1:D:3446:GLY:N	2.29	0.46
1:E:4261:ASN:HA	1:E:4264:ARG:HE	1.80	0.46
1:G:6182:GLY:O	1:G:6185:CYS:SG	2.73	0.46
1:G:6298:ILE:O	1:G:6299:SER:HB2	2.14	0.46
1:H:7279:ASP:N	1:H:7279:ASP:OD1	2.46	0.46
1:A:351:VAL:CG1	1:A:369:ALA:HB2	2.43	0.46
1:B:1349:LEU:O	1:B:1354:ARG:HD2	2.15	0.46
1:C:2417:PHE:CE2	1:C:2444:ALA:HB3	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2481:CYS:SG	1:C:2540:ALA:CB	3.04	0.46
1:C:2484:ARG:C	1:C:2485:HIS:ND1	2.69	0.46
1:D:3075:MSE:CB	1:D:3081:LYS:HD3	2.35	0.46
1:D:3553:VAL:C	1:D:3555:GLU:N	2.69	0.46
1:E:4043:GLN:HG3	1:E:4047:MSE:HE3	1.97	0.46
1:E:4079:LEU:O	1:E:4083:ILE:HG13	2.16	0.46
1:E:4294:ALA:O	1:E:4295:GLN:C	2.53	0.46
1:E:4344:PHE:CD2	1:E:4344:PHE:O	2.68	0.46
1:E:4439:GLY:HA3	1:E:4460:PHE:CE2	2.51	0.46
1:F:5186:LEU:O	1:F:5187:TYR:C	2.52	0.46
1:G:6349:LEU:CD2	1:G:6351:VAL:HG23	2.46	0.46
1:G:6528:ILE:HD13	1:G:6550:ALA:HA	1.97	0.46
1:H:7230:GLN:O	1:H:7233:ASP:HB2	2.14	0.46
1:H:7416:ILE:O	1:H:7443:PHE:HA	2.16	0.46
1:H:7445:SER:O	1:H:7464:GLN:HA	2.16	0.46
1:H:7503:THR:HG23	1:H:7506:GLU:OE1	2.16	0.46
1:H:7511:ARG:CB	1:H:7511:ARG:NH1	2.78	0.46
1:A:177:MSE:O	1:A:181:VAL:HG22	2.16	0.46
1:A:389:ILE:O	1:A:389:ILE:HG23	2.15	0.46
1:A:413:ARG:HH21	1:A:441:CYS:N	2.14	0.46
1:B:1279:ASP:O	1:B:1280:ILE:HG13	2.16	0.46
1:B:1293:ALA:CB	1:B:1512:LEU:HB3	2.46	0.46
1:C:2161:THR:HG22	1:C:2180:PRO:HG3	1.97	0.46
1:C:2156:LYS:O	1:C:2251:LEU:HB3	2.15	0.46
1:C:2471:PHE:CD2	1:C:2472:PRO:HD3	2.50	0.46
1:D:3135:ILE:CD1	1:D:3143:VAL:HG13	2.46	0.46
1:D:3379:ASP:O	1:D:3383:ILE:HG13	2.15	0.46
1:D:3422:PRO:HD2	1:D:3425:GLN:HG2	1.96	0.46
1:D:3529:LYS:O	1:D:3530:VAL:C	2.53	0.46
1:E:4081:LYS:O	1:E:4085:ILE:HG22	2.15	0.46
1:E:4350:LEU:CD1	1:E:4354:ARG:CZ	2.92	0.46
1:E:4373:ILE:HG22	1:E:4373:ILE:O	2.15	0.46
1:E:4472:PRO:HG2	1:E:4523:SER:HB3	1.98	0.46
1:F:5310:LEU:HD21	1:F:5398:LEU:HD22	1.98	0.46
1:F:5508:ALA:C	1:F:5510:GLY:N	2.68	0.46
1:F:5511:ARG:HB2	1:F:5511:ARG:HH11	1.80	0.46
1:G:6528:ILE:HA	1:G:6553:VAL:HG21	1.98	0.46
1:H:7094:LYS:O	1:H:7097:TYR:N	2.48	0.46
1:H:7388:THR:HG22	1:H:7389:ILE:N	2.30	0.46
1:H:7481:CYS:C	1:H:7483:THR:H	2.18	0.46
1:A:219:MSE:HB2	1:B:1038:MSE:SE	2.66	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:LEU:C	1:A:344:PHE:O	2.54	0.46
1:A:389:ILE:HG21	1:A:416:ILE:HG22	1.98	0.46
1:B:1133:LEU:HA	1:B:1133:LEU:HD12	1.68	0.46
1:B:1471:PHE:CD1	1:B:1472:PRO:CD	2.99	0.46
1:C:2210:ILE:HD11	1:C:2224:LYS:NZ	2.30	0.46
1:C:2323:ILE:O	1:C:2324:VAL:C	2.53	0.46
1:C:2327:MSE:CE	1:C:2341:ILE:HD11	2.45	0.46
1:C:2191:ALA:O	1:C:2476:LEU:HD22	2.16	0.46
1:C:2549:LYS:O	1:C:2553:VAL:HG23	2.15	0.46
1:D:3258:GLY:O	1:D:3260:HIS:N	2.49	0.46
1:E:4156:LYS:HG3	1:E:4197:ARG:HB3	1.98	0.46
1:F:5533:TYR:C	1:F:5533:TYR:CD2	2.88	0.46
1:G:6184:LEU:HG	1:G:6198:CYS:HB3	1.97	0.46
1:G:6223:GLN:HG2	1:G:6224:LYS:N	2.30	0.46
1:G:6300:LYS:NZ	1:G:6304:GLU:HB2	2.31	0.46
1:G:6314:GLU:CG	1:G:6315:ALA:H	2.29	0.46
1:G:6477:ALA:O	1:G:6481:CYS:HB2	2.16	0.46
1:G:6536:ALA:HA	1:G:6538:LYS:HZ3	1.79	0.46
1:H:7140:ARG:HG3	1:H:7140:ARG:O	2.15	0.46
1:A:137:ILE:HA	1:A:234:LEU:CD2	2.45	0.46
1:A:453:LYS:CD	1:A:457:GLY:HA2	2.43	0.46
1:B:1321:ASN:O	1:B:1324:VAL:N	2.49	0.46
1:C:2069:HIS:C	1:C:2071:ASN:N	2.67	0.46
1:C:2232:ASP:O	1:C:2235:ILE:HG12	2.16	0.46
1:C:2300:LYS:HD3	1:C:2305:HIS:CD2	2.51	0.46
1:C:2156:LYS:CB	1:C:2479:ILE:HD13	2.44	0.46
1:D:3243:THR:HB	1:D:3248:ARG:NH1	2.31	0.46
1:D:3376:THR:HG22	1:D:3377:PHE:N	2.29	0.46
1:D:3533:TYR:CD2	1:D:3533:TYR:C	2.89	0.46
1:E:4104:ILE:HG23	1:E:4105:GLU:H	1.81	0.46
1:E:4177:MSE:O	1:E:4181:VAL:HG23	2.15	0.46
1:F:5351:VAL:HG22	1:F:5369:ALA:HA	1.98	0.46
1:G:6024:LYS:C	1:G:6028:LEU:HD22	2.36	0.46
1:G:6238:PHE:O	1:G:6239:MSE:C	2.53	0.46
1:G:6282:GLY:O	1:G:6283:THR:C	2.54	0.46
1:A:238:PHE:O	1:A:242:ILE:HG12	2.16	0.46
1:A:483:THR:HG23	1:A:539:MSE:O	2.16	0.46
1:A:45:ARG:NH1	1:A:58:ILE:HD13	2.31	0.46
1:B:1090:GLU:HG2	1:B:1131:LYS:HZ2	1.80	0.46
1:B:1137:ILE:O	1:B:1137:ILE:HG13	2.15	0.46
1:B:1326:SER:O	1:B:1327:MSE:C	2.53	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1326:SER:O	1:B:1329:GLU:N	2.49	0.46
1:C:2025:GLY:O	1:C:2028:LEU:HB2	2.15	0.46
1:C:2132:GLY:HA3	1:C:2177:MSE:HE1	1.97	0.46
1:C:2261:ASN:HA	1:C:2264:ARG:NE	2.31	0.46
1:C:2302:ILE:HD12	1:C:2302:ILE:H	1.80	0.46
1:C:2360:SER:HA	1:C:2363:GLU:OE1	2.15	0.46
1:C:2458:ARG:HH11	1:C:2458:ARG:HB2	1.80	0.46
1:D:3194:ARG:HH21	1:D:3197:ARG:HE	1.64	0.46
1:D:3309:PHE:HD1	1:D:3390:ILE:HB	1.79	0.46
1:E:4321:ASN:C	1:E:4321:ASN:OD1	2.54	0.46
1:E:4470:ILE:HD11	1:E:4498:LEU:HD23	1.98	0.46
1:F:5333:SER:HB3	1:F:5336:GLU:CD	2.36	0.46
1:G:6230:GLN:O	1:G:6233:ASP:HB2	2.16	0.46
1:G:6401:PRO:O	1:G:6405:ARG:HG2	2.16	0.46
1:H:7358:ILE:HG21	1:H:7366:THR:OG1	2.16	0.46
1:H:7394:GLY:HA2	1:H:7420:SER:CB	2.41	0.46
1:H:7429:THR:HG23	1:H:7432:GLU:CG	2.46	0.46
1:H:7434:TYR:CG	1:H:7460:PHE:HD2	2.34	0.46
1:H:7498:LEU:O	1:H:7501:GLN:CB	2.57	0.46
1:H:7499:THR:O	1:H:7502:LEU:HB2	2.16	0.46
1:A:150:TRP:CE2	1:A:199:LEU:HD13	2.51	0.46
1:A:236:ASP:O	1:A:237:GLU:C	2.53	0.46
1:A:261:ASN:HA	1:A:264:ARG:HG2	1.98	0.46
1:A:44:GLU:O	1:A:48:LEU:N	2.46	0.46
1:B:1164:GLU:HG3	1:B:1171:ASP:OD2	2.16	0.46
1:C:2039:ALA:HA	1:C:2059:GLU:O	2.16	0.46
1:C:2320:ALA:HB1	1:C:2365:PHE:CE2	2.51	0.46
1:D:3082:TYR:HA	1:D:3085:ILE:HG22	1.98	0.46
1:D:3169:LEU:HD22	1:D:3172:LEU:HD11	1.98	0.46
1:D:3183:LYS:CD	1:D:3255:GLU:OE2	2.64	0.46
1:D:3186:LEU:O	1:D:3187:TYR:C	2.54	0.46
1:D:3321:ASN:O	1:D:3324:VAL:HB	2.15	0.46
1:E:4037:GLY:C	1:E:4039:ALA:N	2.68	0.46
1:E:4093:GLU:O	1:E:4096:PHE:HB3	2.16	0.46
1:E:4229:GLN:O	1:E:4232:ASP:N	2.49	0.46
1:E:4243:THR:HG22	1:E:4247:GLY:O	2.16	0.46
1:G:6112:TYR:CE2	1:G:6113:THR:HG23	2.51	0.46
1:H:7081:LYS:O	1:H:7085:ILE:HG22	2.16	0.46
1:H:7083:ILE:HD11	1:H:7126:ILE:HG21	1.96	0.46
1:H:7401:PRO:O	1:H:7405:ARG:HG2	2.16	0.46
1:A:184:LEU:HG	1:A:198:CYS:CB	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:GLU:OE2	1:A:278:ASP:HB3	2.15	0.45
1:A:285:ALA:HA	1:A:322:LEU:HD22	1.98	0.45
1:A:453:LYS:HG2	1:A:458:ARG:N	2.31	0.45
1:B:1108:MSE:N	1:B:1109:PRO:HD2	2.31	0.45
1:B:1307:ILE:HG12	1:B:1388:THR:CB	2.41	0.45
1:B:1390:ILE:HG23	1:B:1419:LEU:HD21	1.97	0.45
1:C:2177:MSE:O	1:C:2177:MSE:HG3	2.16	0.45
1:E:4115:THR:O	1:E:4118:LEU:N	2.49	0.45
1:E:4164:GLU:O	1:E:4171:ASP:N	2.49	0.45
1:E:4408:ALA:HA	1:E:4414:PRO:HG3	1.98	0.45
1:F:5258:GLY:O	1:F:5259:ASN:C	2.54	0.45
1:F:5363:GLU:O	1:F:5365:PHE:N	2.50	0.45
1:H:7243:THR:HG22	1:H:7248:ARG:HA	1.98	0.45
1:A:85:ILE:C	1:A:87:GLY:N	2.69	0.45
1:A:61:GLN:HG2	1:A:98:ARG:HD3	1.97	0.45
1:A:99:ILE:O	1:A:102:ASP:HB2	2.16	0.45
1:B:1431:GLU:C	1:B:1433:ALA:N	2.70	0.45
1:D:3184:LEU:O	1:D:3185:CYS:C	2.53	0.45
1:D:3464:GLN:O	1:D:3469:TYR:HE1	2.00	0.45
1:D:3527:ALA:O	1:D:3528:ILE:C	2.52	0.45
1:E:4033:ARG:NE	1:E:4093:GLU:OE1	2.49	0.45
1:E:4124:GLY:O	1:E:4217:PHE:HB3	2.15	0.45
1:E:4543:TYR:CD2	1:E:4543:TYR:C	2.89	0.45
1:F:5240:LYS:HG2	1:F:5244:ASP:CG	2.36	0.45
1:G:6219:MSE:HE3	1:G:6219:MSE:HB2	1.94	0.45
1:G:6478:VAL:HG21	1:G:6486:ILE:HD13	1.98	0.45
1:G:6504:ASP:HA	1:G:6507:LEU:HB2	1.99	0.45
1:A:258:GLY:O	1:A:259:ASN:C	2.55	0.45
1:A:267:ARG:HH11	1:A:267:ARG:CG	2.24	0.45
1:A:324:VAL:O	1:A:325:MSE:C	2.53	0.45
1:A:493:GLU:HG3	1:A:494:ALA:N	2.31	0.45
1:B:1306:LYS:CD	1:B:1384:LEU:O	2.64	0.45
1:B:1420:SER:CB	1:B:1427:GLU:OE1	2.64	0.45
1:B:1454:LEU:O	1:B:1457:GLY:N	2.49	0.45
1:C:2136:SER:O	1:C:2139:ASP:HB2	2.17	0.45
1:C:2179:ILE:O	1:C:2180:PRO:C	2.55	0.45
1:C:2210:ILE:O	1:C:2214:LYS:HG3	2.16	0.45
1:C:2174:VAL:CG2	1:C:2219:MSE:HE3	2.47	0.45
1:C:2240:LYS:HG3	1:C:2248:ARG:HH22	1.80	0.45
1:C:2520:GLN:HB2	1:C:2521:GLU:H	1.67	0.45
1:E:4143:VAL:O	1:E:4146:ILE:HB	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:4332:LEU:HD21	1:E:4340:LYS:NZ	2.31	0.45
1:F:5027:PRO:HA	1:F:5030:LEU:HB2	1.98	0.45
1:G:6033:ARG:NH2	1:G:6196:ASP:HA	2.30	0.45
1:G:6276:PHE:CD1	1:G:6277:ASN:N	2.85	0.45
1:G:6548:ASP:O	1:G:6552:TYR:HB2	2.16	0.45
1:H:7317:LEU:HD21	1:H:7362:GLN:HG3	1.98	0.45
1:H:7339:LYS:HA	1:H:7367:HIS:CE1	2.51	0.45
1:H:7504:ASP:HA	1:H:7507:LEU:HB2	1.97	0.45
1:A:281:GLN:HB3	1:A:491:PHE:CE2	2.52	0.45
1:A:319:ILE:O	1:A:320:ALA:C	2.54	0.45
1:A:469:TYR:HB3	1:A:498:LEU:CD2	2.47	0.45
1:B:1031:ASN:HB3	1:B:1034:THR:OG1	2.17	0.45
1:C:2105:GLU:HA	1:C:2108:MSE:HE3	1.98	0.45
1:C:2528:ILE:O	1:C:2531:THR:N	2.49	0.45
1:D:3239:MSE:O	1:D:3240:LYS:C	2.54	0.45
1:D:3310:LEU:HD21	1:D:3398:LEU:HB2	1.98	0.45
1:D:3419:LEU:HA	1:D:3446:GLY:H	1.81	0.45
1:E:4113:THR:CA	1:E:4116:VAL:HG12	2.38	0.45
1:E:4332:LEU:CD2	1:E:4340:LYS:HD2	2.46	0.45
1:E:4404:ILE:O	1:E:4407:MSE:N	2.50	0.45
1:E:4416:ILE:C	1:E:4417:PHE:HD1	2.19	0.45
1:F:5228:THR:HG1	1:F:5230:GLN:H	1.62	0.45
1:F:5419:LEU:O	1:F:5420:SER:C	2.54	0.45
1:G:6113:THR:CA	1:G:6116:VAL:HG12	2.46	0.45
1:G:6174:VAL:HG23	1:G:6174:VAL:O	2.15	0.45
1:G:6363:GLU:HB2	1:G:6364:PRO:HD3	1.97	0.45
1:H:7089:GLN:HB2	1:H:7096:PHE:CD1	2.51	0.45
1:H:7270:ARG:HA	1:H:7275:THR:HG23	1.98	0.45
1:H:7396:GLY:HA2	1:H:7425:GLN:C	2.37	0.45
1:H:7431:GLU:C	1:H:7433:ALA:N	2.67	0.45
1:A:166:ILE:HD13	1:A:166:ILE:HA	1.77	0.45
1:A:502:LEU:HD12	1:A:506:GLU:HB3	1.98	0.45
1:A:518:ASN:OD1	1:A:518:ASN:N	2.45	0.45
1:A:549:LYS:O	1:A:552:TYR:HB3	2.17	0.45
1:B:1172:LEU:HD23	1:B:1172:LEU:HA	1.68	0.45
1:B:1188:THR:HG23	1:B:1193:ILE:O	2.17	0.45
1:B:1452:VAL:HG12	1:B:1452:VAL:O	2.16	0.45
1:B:1467:ASN:N	1:B:1467:ASN:OD1	2.49	0.45
1:C:2503:THR:O	1:C:2507:LEU:HD22	2.16	0.45
1:D:3108:MSE:CB	1:D:3109:PRO:HD3	2.46	0.45
1:D:3156:LYS:O	1:D:3251:LEU:HB3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3454:LEU:HD11	1:D:3460:PHE:CE2	2.51	0.45
1:E:4325:MSE:HE3	1:E:4325:MSE:HB3	1.92	0.45
1:E:4332:LEU:CB	1:E:4336:GLU:OE2	2.65	0.45
1:E:4395:ALA:HB3	1:E:4398:LEU:HD22	1.99	0.45
1:E:4482:ASN:HA	1:E:4482:ASN:HD22	1.56	0.45
1:E:4565:LEU:HA	1:E:4565:LEU:HD23	1.82	0.45
1:F:5342:TRP:CE3	1:F:5349:LEU:HD11	2.51	0.45
1:F:5374:PRO:HB3	1:F:5383:ILE:HD11	1.99	0.45
1:G:6056:PRO:HB2	1:H:7221:LEU:CD1	2.47	0.45
1:G:6128:ARG:NH1	1:G:6128:ARG:HG2	2.24	0.45
1:H:7082:TYR:O	1:H:7086:MSE:HB2	2.16	0.45
1:H:7319:ILE:O	1:H:7320:ALA:C	2.55	0.45
1:A:135:ILE:O	1:A:203:ILE:HA	2.16	0.45
1:A:26:LYS:N	1:A:27:PRO:HD2	2.31	0.45
1:A:337:ALA:O	1:A:340:LYS:HB2	2.16	0.45
1:A:541:PHE:CD2	1:A:541:PHE:N	2.85	0.45
1:B:1434:TYR:CZ	1:B:1443:PHE:HB3	2.52	0.45
1:C:2038:MSE:C	1:C:2040:PHE:H	2.20	0.45
1:C:2311:GLY:HA2	1:C:2345:ASP:HA	1.99	0.45
1:C:2528:ILE:HB	1:C:2529:LYS:H	1.63	0.45
1:D:3177:MSE:CE	1:D:3180:PRO:HB2	2.46	0.45
1:D:3270:ARG:CG	1:D:3271:GLU:N	2.78	0.45
1:D:3431:GLU:O	1:D:3435:THR:HG23	2.17	0.45
1:D:3487:SER:O	1:D:3490:VAL:HB	2.16	0.45
1:F:5093:GLU:O	1:F:5096:PHE:N	2.50	0.45
1:F:5108:MSE:HE2	1:F:5108:MSE:HB2	1.68	0.45
1:F:5458:ARG:HH11	1:F:5458:ARG:CB	2.30	0.45
1:F:5537:ASN:N	1:F:5537:ASN:ND2	2.64	0.45
1:H:7454:LEU:CD1	1:H:7458:ARG:HB2	2.47	0.45
1:A:303:SER:HA	1:A:340:LYS:HZ1	1.82	0.45
1:A:504:ASP:O	1:A:507:LEU:HB2	2.17	0.45
1:B:1376:THR:HG22	1:B:1379:ASP:N	2.26	0.45
1:C:2045:ARG:O	1:C:2051:GLN:N	2.50	0.45
1:C:2085:ILE:HG23	1:C:2086:MSE:N	2.32	0.45
1:C:2328:VAL:C	1:C:2330:ASN:H	2.19	0.45
1:C:2390:ILE:CG2	1:C:2419:LEU:HD21	2.47	0.45
1:D:3194:ARG:NH2	1:D:3196:ASP:OD2	2.50	0.45
1:D:3264:ARG:CG	1:D:3265:PHE:N	2.80	0.45
1:D:3275:THR:OG1	1:D:3276:PHE:N	2.48	0.45
1:E:4082:TYR:O	1:E:4085:ILE:HG22	2.17	0.45
1:E:4300:LYS:O	1:E:4302:ILE:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:5137:ILE:C	1:F:5139:ASP:H	2.20	0.45
1:F:5393:ALA:HB1	3:F:5601:NAD:C4A	2.47	0.45
1:G:6146:ILE:O	1:G:6149:ASN:N	2.36	0.45
1:G:6419:LEU:HD22	1:G:6419:LEU:H	1.81	0.45
1:H:7166:ILE:CD1	1:H:7176:GLY:HA3	2.46	0.45
1:H:7417:PHE:CD2	1:H:7444:ALA:HB3	2.52	0.45
1:A:231:TYR:O	1:A:235:ILE:HG12	2.17	0.45
1:A:342:TRP:CZ3	1:A:367:HIS:HB2	2.52	0.45
1:A:419:LEU:HA	1:A:446:GLY:N	2.27	0.45
1:A:555:GLU:HB3	1:A:556:ARG:NH1	2.31	0.45
1:B:1370:PRO:O	1:B:1371:GLU:C	2.55	0.45
1:B:1570:TYR:N	1:B:1570:TYR:CD2	2.84	0.45
1:C:2061:GLN:HA	1:C:2064:GLN:NE2	2.26	0.45
1:C:2301:PRO:O	1:C:2302:ILE:C	2.54	0.45
1:C:2412:GLU:C	1:C:2413:ARG:HG2	2.35	0.45
1:C:2394:GLY:HA2	1:C:2420:SER:OG	2.17	0.45
1:D:3150:TRP:CE3	1:D:3151:PRO:HD2	2.50	0.45
1:D:3229:GLN:O	1:D:3230:GLN:C	2.55	0.45
1:D:3300:LYS:O	1:D:3305:HIS:CE1	2.69	0.45
1:D:3511:ARG:HH11	1:D:3511:ARG:HB2	1.81	0.45
1:F:5093:GLU:O	1:F:5094:LYS:C	2.55	0.45
1:F:5144:ARG:HH12	1:F:5245:ARG:N	2.15	0.45
1:F:5242:ILE:O	1:F:5243:THR:C	2.55	0.45
1:F:5338:GLN:HB3	1:F:5338:GLN:HE21	1.54	0.45
1:F:5471:PHE:CD1	1:F:5472:PRO:HD3	2.51	0.45
1:F:5494:ALA:O	1:F:5498:LEU:N	2.35	0.45
1:G:6031:ASN:HA	1:G:6032:PRO:HD2	1.72	0.45
1:G:6063:ILE:O	1:G:6066:LEU:HB3	2.17	0.45
1:G:6173:GLY:HA3	1:G:6218:TYR:OH	2.16	0.45
1:G:6300:LYS:HZ2	1:G:6304:GLU:C	2.20	0.45
1:H:7026:LYS:HD2	1:H:7029:MSE:CE	2.47	0.45
1:H:7143:VAL:HG11	1:H:7238:PHE:HA	1.98	0.45
1:H:7422:PRO:C	1:H:7424:ALA:N	2.66	0.45
1:H:7552:TYR:HE1	1:H:7556:ARG:CZ	2.30	0.45
1:A:210:ILE:HG22	1:A:214:LYS:CD	2.43	0.45
1:A:360:SER:HA	1:A:363:GLU:HG3	1.99	0.45
1:B:1085:ILE:O	1:B:1085:ILE:HG13	2.16	0.45
1:B:1103:ASP:HB3	1:B:1107:LEU:CD2	2.46	0.45
1:B:1359:ASP:OD2	1:B:1362:GLN:HB2	2.17	0.45
1:C:2164:GLU:HG3	1:C:2225:ARG:CZ	2.46	0.45
1:C:2243:THR:HG22	1:C:2248:ARG:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2416:ILE:HD11	1:C:2443:PHE:HB2	1.99	0.45
1:C:2390:ILE:HG23	1:C:2419:LEU:HD21	1.98	0.45
1:D:3377:PHE:HZ	1:D:3389:ILE:CD1	2.26	0.45
1:E:4291:LEU:N	1:E:4291:LEU:HD23	2.31	0.45
1:E:4317:LEU:H	1:E:4317:LEU:CD1	2.26	0.45
1:E:4402:ASP:HA	1:E:4405:ARG:CG	2.43	0.45
1:F:5057:LYS:O	1:F:5058:ILE:HD13	2.15	0.45
1:F:5255:GLU:O	1:F:5256:ASP:C	2.54	0.45
1:G:6061:GLN:HA	1:G:6064:GLN:HE21	1.82	0.45
1:G:6210:ILE:HG22	1:G:6214:LYS:CE	2.43	0.45
1:G:6240:LYS:O	1:G:6244:ASP:HB2	2.17	0.45
1:G:6385:LYS:N	1:G:6386:PRO:CD	2.80	0.45
1:H:7035:ASN:OD1	1:H:7036:LYS:N	2.50	0.45
1:H:7224:LYS:HA	1:H:7224:LYS:HD2	1.77	0.45
1:H:7183:LYS:NZ	1:H:7255:GLU:OE2	2.47	0.45
1:H:7326:SER:HA	1:H:7329:GLU:HG2	1.99	0.45
1:H:7333:SER:HB3	1:H:7336:GLU:CD	2.37	0.45
1:H:7335:GLN:O	1:H:7335:GLN:NE2	2.50	0.45
1:H:7302:ILE:HG22	1:H:7340:LYS:NZ	2.31	0.45
1:H:7108:MSE:HE3	1:H:7516:LEU:HD23	1.97	0.45
1:A:288:LEU:O	1:A:289:ALA:C	2.55	0.45
1:A:291:LEU:HD23	1:A:417:PHE:CZ	2.52	0.45
1:A:417:PHE:CD2	1:A:444:ALA:HB3	2.51	0.45
1:A:55:PRO:O	1:A:57:LYS:N	2.50	0.45
1:B:1370:PRO:HD2	1:B:1373:ILE:CD1	2.47	0.45
1:B:1559:ARG:HD3	1:B:1559:ARG:HA	1.40	0.45
1:C:2146:ILE:O	1:C:2149:ASN:HB2	2.16	0.45
1:C:2160:VAL:CG1	1:C:2201:VAL:HB	2.45	0.45
1:C:2403:VAL:O	1:C:2404:ILE:C	2.54	0.45
1:C:2481:CYS:SG	1:C:2540:ALA:HB1	2.57	0.45
1:D:3414:PRO:O	1:D:3442:LEU:HD12	2.16	0.45
1:D:3511:ARG:CB	1:D:3511:ARG:HH11	2.29	0.45
1:E:4337:ALA:HA	1:E:4340:LYS:HD2	1.99	0.45
1:F:5384:LEU:O	1:F:5385:LYS:C	2.55	0.45
1:G:6300:LYS:C	1:G:6304:GLU:OE1	2.56	0.45
1:H:7085:ILE:HG23	1:H:7086:MSE:N	2.32	0.45
1:H:7109:PRO:O	1:H:7114:PRO:HD2	2.17	0.45
1:H:7268:LYS:HG2	1:H:7269:TYR:CZ	2.52	0.45
1:H:7389:ILE:O	1:H:7389:ILE:HG23	2.15	0.45
1:A:158:VAL:CG1	1:A:159:VAL:N	2.80	0.44
1:A:154:HIS:HB3	1:A:197:ARG:NE	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:GLU:HG2	1:A:363:GLU:H	1.51	0.44
1:A:81:LYS:O	1:A:85:ILE:HG22	2.17	0.44
1:B:1108:MSE:HB2	1:B:1108:MSE:HE2	1.69	0.44
1:B:1270:ARG:CG	1:B:1271:GLU:N	2.79	0.44
1:B:1274:CYS:O	1:B:1486:ILE:HD11	2.17	0.44
1:C:2249:ASN:OD1	1:C:2249:ASN:C	2.55	0.44
1:C:2283:THR:O	1:C:2285:ALA:N	2.50	0.44
1:C:2374:PRO:HG3	1:C:2380:ALA:HA	1.99	0.44
1:C:2377:PHE:HZ	1:C:2389:ILE:CD1	2.30	0.44
1:D:3302:ILE:HG22	1:D:3340:LYS:NZ	2.32	0.44
1:E:4300:LYS:HB3	1:E:4305:HIS:NE2	2.32	0.44
1:E:4402:ASP:HA	1:E:4405:ARG:HD2	1.98	0.44
1:E:4530:VAL:O	1:E:4533:TYR:HB3	2.17	0.44
1:F:5346:LYS:HE3	1:F:5346:LYS:HB2	1.34	0.44
1:F:5359:ASP:OD2	1:F:5361:TYR:HB2	2.16	0.44
1:F:5452:VAL:O	1:F:5460:PHE:N	2.43	0.44
1:F:5469:TYR:O	1:F:5470:ILE:HD13	2.16	0.44
1:F:5495:ALA:O	1:F:5498:LEU:HB3	2.16	0.44
1:G:6416:ILE:HD12	1:G:6441:CYS:HB2	1.98	0.44
1:H:7132:GLY:HA3	1:H:7177:MSE:CE	2.47	0.44
1:H:7239:MSE:HE2	1:H:7269:TYR:CD1	2.52	0.44
1:H:7412:GLU:O	1:H:7440:ARG:HD2	2.16	0.44
1:H:7414:PRO:HD2	1:H:7440:ARG:O	2.16	0.44
1:A:332:LEU:CD2	1:A:337:ALA:HA	2.46	0.44
1:A:431:GLU:C	1:A:433:ALA:N	2.71	0.44
1:A:416:ILE:HD12	1:A:441:CYS:HB2	1.99	0.44
1:A:534:LEU:HD23	1:A:539:MSE:HB2	1.99	0.44
1:B:1552:TYR:HE1	1:B:1556:ARG:CZ	2.30	0.44
1:C:2478:VAL:HG13	1:C:2483:THR:HB	1.99	0.44
1:C:2520:GLN:O	1:C:2521:GLU:C	2.54	0.44
1:D:3054:LEU:O	1:D:3055:PRO:C	2.56	0.44
1:D:3300:LYS:HZ3	1:D:3304:GLU:HB2	1.82	0.44
1:D:3419:LEU:O	1:D:3420:SER:C	2.54	0.44
1:D:3453:LYS:HA	1:D:3459:VAL:CG1	2.47	0.44
1:E:4075:MSE:HB2	1:E:4075:MSE:HE3	1.76	0.44
1:F:5148:ASP:HA	1:F:5245:ARG:HH11	1.82	0.44
1:F:5315:ALA:C	1:F:5319:ILE:HD12	2.38	0.44
1:G:6343:MSE:O	1:G:6350:LEU:HB2	2.17	0.44
1:H:7166:ILE:HD11	1:H:7176:GLY:HA3	1.99	0.44
1:H:7380:ALA:O	1:H:7381:VAL:C	2.54	0.44
1:A:233:ASP:N	1:A:233:ASP:OD1	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:377:PHE:HZ	1:A:389:ILE:CD1	2.26	0.44
1:A:38:MSE:O	1:A:58:ILE:HA	2.17	0.44
1:B:1335:GLN:HG3	1:B:1336:GLU:N	2.31	0.44
1:B:1360:SER:HA	1:B:1363:GLU:OE1	2.18	0.44
1:B:1531:THR:O	1:B:1532:GLU:C	2.55	0.44
1:C:2219:MSE:HB2	1:C:2219:MSE:HE3	1.89	0.44
1:D:3204:ASP:OD1	1:D:3221:LEU:CD2	2.66	0.44
1:D:3376:THR:O	1:D:3379:ASP:HB2	2.17	0.44
1:D:3306:LYS:HB3	1:D:3386:PRO:HA	1.99	0.44
1:D:3428:CYS:SG	1:D:3429:THR:N	2.91	0.44
1:D:3533:TYR:O	1:D:3536:ALA:HB3	2.18	0.44
1:F:5029:MSE:SE	1:F:5050:LEU:HD22	2.68	0.44
1:F:5179:ILE:HG12	1:F:5179:ILE:H	1.57	0.44
1:F:5376:THR:CG2	1:F:5378:GLU:HB3	2.48	0.44
1:G:6133:LEU:HD13	1:G:6150:TRP:HE3	1.83	0.44
1:H:7143:VAL:O	1:H:7146:ILE:HB	2.18	0.44
1:H:7288:LEU:C	1:H:7290:GLY:N	2.70	0.44
1:H:7429:THR:HG23	1:H:7432:GLU:HG3	1.99	0.44
1:H:7419:LEU:HA	1:H:7446:GLY:N	2.32	0.44
1:H:7322:LEU:HD11	1:H:7492:LEU:CA	2.48	0.44
1:A:243:THR:HG21	1:A:273:TYR:HD2	1.82	0.44
1:A:476:LEU:HD12	1:A:480:LEU:HD11	1.98	0.44
1:B:1250:THR:O	1:B:1250:THR:HG23	2.18	0.44
1:B:1335:GLN:HE22	1:B:1339:LYS:HG3	1.78	0.44
1:B:1346:LYS:HB3	3:B:1601:NAD:C5A	2.48	0.44
1:C:2127:PHE:CD1	1:C:2219:MSE:SE	3.21	0.44
1:C:2266:LEU:HD21	1:C:2281:GLN:HE21	1.82	0.44
1:C:2419:LEU:HA	1:C:2446:GLY:HA3	1.99	0.44
1:C:2452:VAL:O	1:C:2460:PHE:N	2.40	0.44
1:E:4086:MSE:CE	1:E:4111:VAL:HG22	2.47	0.44
1:E:4209:ASN:C	1:E:4209:ASN:OD1	2.55	0.44
1:E:4281:GLN:HE21	1:E:4491:PHE:HE1	1.66	0.44
1:E:4553:VAL:C	1:E:4555:GLU:N	2.70	0.44
1:F:5104:ILE:HG13	1:F:5108:MSE:CE	2.48	0.44
1:F:5266:LEU:CD2	1:F:5281:GLN:OE1	2.65	0.44
1:F:5283:THR:O	1:F:5285:ALA:N	2.50	0.44
1:G:6240:LYS:O	1:G:6241:ALA:C	2.55	0.44
1:G:6404:ILE:HB	1:G:6436:LEU:CD2	2.36	0.44
1:G:6466:ASN:CG	1:G:6468:VAL:HG12	2.38	0.44
1:H:7243:THR:CB	1:H:7248:ARG:NH1	2.81	0.44
1:A:503:THR:H	1:A:506:GLU:HB2	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:393:ALA:HB1	3:A:601:NAD:C4A	2.48	0.44
1:B:1516:LEU:HA	1:B:1516:LEU:HD12	1.81	0.44
1:B:1537:ASN:N	1:B:1537:ASN:ND2	2.64	0.44
1:B:1540:ALA:C	1:B:1541:PHE:HD2	2.20	0.44
1:C:2140:ARG:HE	1:C:2140:ARG:HB2	1.47	0.44
1:C:2295:GLN:HE22	1:C:2305:HIS:CE1	2.35	0.44
1:C:2300:LYS:HA	1:C:2301:PRO:HD2	1.81	0.44
1:C:2370:PRO:HD2	1:C:2373:ILE:HD12	1.95	0.44
1:C:2454:LEU:HD13	1:C:2458:ARG:NH1	2.31	0.44
1:D:3122:GLN:HA	1:D:3122:GLN:NE2	2.31	0.44
1:D:3245:ARG:HG2	1:D:3245:ARG:O	2.18	0.44
1:D:3243:THR:CB	1:D:3248:ARG:NH1	2.80	0.44
1:D:3290:GLY:O	1:D:3293:ALA:HB3	2.18	0.44
1:D:3375:ASP:OD2	1:D:3376:THR:N	2.49	0.44
1:D:3481:CYS:SG	1:D:3540:ALA:HB1	2.57	0.44
1:D:3506:GLU:O	1:D:3511:ARG:HG3	2.17	0.44
1:E:4358:ILE:HG12	1:E:4366:THR:HG21	2.00	0.44
1:F:5029:MSE:HE2	1:F:5029:MSE:HB2	1.90	0.44
1:F:5055:PRO:O	1:F:5057:LYS:N	2.46	0.44
1:F:5501:GLN:OE1	1:F:5525:ASN:HB3	2.17	0.44
1:G:6478:VAL:HG22	1:G:6483:THR:HB	2.00	0.44
1:H:7024:LYS:HD3	1:H:7048:LEU:O	2.17	0.44
1:A:341:ILE:HB	1:A:365:PHE:HD2	1.83	0.44
1:A:431:GLU:C	1:A:433:ALA:H	2.20	0.44
1:A:471:PHE:CE1	1:A:472:PRO:HG3	2.53	0.44
1:A:503:THR:HG23	1:A:506:GLU:OE1	2.18	0.44
1:B:1193:ILE:HG22	1:B:1198:CYS:SG	2.58	0.44
1:B:1259:ASN:HB2	1:B:1260:HIS:H	1.44	0.44
1:B:1270:ARG:HH21	1:B:1487:SER:HA	1.83	0.44
1:B:1503:THR:HB	1:B:1505:GLU:OE1	2.18	0.44
1:C:2026:LYS:C	1:C:2028:LEU:N	2.71	0.44
1:C:2099:ILE:O	1:C:2102:ASP:HB2	2.17	0.44
1:C:2255:GLU:OE1	1:C:2256:ASP:N	2.49	0.44
1:C:2309:PHE:CE1	1:C:2390:ILE:HB	2.51	0.44
1:C:2403:VAL:HG12	1:C:2404:ILE:N	2.32	0.44
1:C:2392:VAL:CG2	1:C:2419:LEU:HD23	2.48	0.44
1:D:3119:ALA:O	1:D:3120:CYS:C	2.55	0.44
1:D:3159:VAL:HA	1:D:3253:GLN:O	2.17	0.44
1:D:3385:LYS:HB2	1:D:3385:LYS:HE3	1.67	0.44
1:D:3389:ILE:HD12	1:D:3389:ILE:HA	1.76	0.44
1:D:3506:GLU:CB	1:D:3511:ARG:HD2	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:4095:LEU:O	1:E:4096:PHE:C	2.56	0.44
1:E:4240:LYS:O	1:E:4241:ALA:C	2.55	0.44
1:F:5197:ARG:CG	1:F:5197:ARG:HH11	2.30	0.44
1:F:5402:ASP:OD1	1:F:5402:ASP:N	2.51	0.44
1:F:5418:ALA:O	1:F:5446:GLY:N	2.48	0.44
1:F:5566:LEU:HD23	1:F:5566:LEU:HA	1.85	0.44
1:G:6370:PRO:HD2	1:G:6373:ILE:HD11	2.00	0.44
1:G:6525:ASN:HA	1:G:6528:ILE:HG13	2.00	0.44
1:A:147:VAL:HG21	1:A:241:ALA:HB1	1.98	0.44
1:A:209:ASN:O	1:A:213:LEU:HG	2.17	0.44
1:A:259:ASN:N	1:A:259:ASN:ND2	2.66	0.44
1:A:295:GLN:NE2	1:A:305:HIS:CE1	2.84	0.44
1:A:82:TYR:HA	1:A:85:ILE:CG2	2.48	0.44
1:B:1207:THR:HG23	1:B:1213:LEU:CD2	2.45	0.44
1:B:1210:ILE:O	1:B:1211:ALA:C	2.56	0.44
1:B:1389:ILE:HA	1:B:1389:ILE:HD12	1.84	0.44
1:B:1401:PRO:CB	1:B:1436:LEU:HD21	2.48	0.44
1:C:2308:LEU:HD13	1:C:2342:TRP:CB	2.48	0.44
1:D:3277:ASN:OD1	1:D:3278:ASP:N	2.51	0.44
1:D:3421:ASN:CA	1:D:3422:PRO:O	2.49	0.44
1:E:4146:ILE:HG23	1:F:5052:GLY:HA3	2.00	0.44
1:E:4496:LYS:H	1:E:4496:LYS:HG3	1.58	0.44
1:F:5288:LEU:C	1:F:5290:GLY:N	2.70	0.44
1:F:5302:ILE:HB	1:F:5303:SER:H	1.47	0.44
1:F:5402:ASP:HA	1:F:5405:ARG:HD2	1.99	0.44
1:F:5453:LYS:HE3	1:F:5457:GLY:CA	2.35	0.44
1:G:6182:GLY:CA	1:G:6185:CYS:SG	3.05	0.44
1:G:6253:GLN:HG3	1:G:6276:PHE:CE1	2.53	0.44
1:G:6363:GLU:CB	1:G:6364:PRO:CD	2.96	0.44
1:G:6437:THR:O	1:G:6440:ARG:HB2	2.17	0.44
1:G:6487:SER:O	1:G:6488:ASP:C	2.53	0.44
1:H:7228:THR:OG1	1:H:7230:GLN:CG	2.65	0.44
1:H:7382:ASN:O	1:H:7385:LYS:HE2	2.18	0.44
1:A:374:PRO:HG3	1:A:380:ALA:HA	1.99	0.44
1:A:476:LEU:HD12	1:A:476:LEU:C	2.37	0.44
1:A:542:ARG:NE	1:A:552:TYR:OH	2.51	0.44
1:B:1184:LEU:O	1:B:1187:TYR:HB2	2.17	0.44
1:B:1338:GLN:O	1:B:1341:ILE:N	2.43	0.44
1:B:1381:VAL:HG13	1:B:1407:MSE:HE1	2.00	0.44
1:B:1466:ASN:CB	1:B:1468:VAL:HG12	2.35	0.44
1:C:2068:PHE:CZ	1:C:2072:LEU:HD22	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2350:LEU:HD12	1:C:2366:THR:HG23	1.98	0.44
1:C:2559:ARG:HG3	1:C:2561:GLU:HG2	1.99	0.44
1:D:3038:MSE:HA	1:D:3045:ARG:HH21	1.82	0.44
1:D:3058:ILE:H	1:D:3058:ILE:HG12	1.53	0.44
1:D:3143:VAL:O	1:D:3146:ILE:N	2.50	0.44
1:D:3258:GLY:O	1:D:3261:ASN:N	2.51	0.44
1:D:3400:THR:C	1:D:3402:ASP:N	2.71	0.44
1:D:3429:THR:C	1:D:3431:GLU:H	2.21	0.44
1:E:4086:MSE:HE3	1:E:4111:VAL:HG22	2.00	0.44
1:F:5100:LEU:HA	1:F:5100:LEU:HD12	1.65	0.44
1:F:5284:ALA:HA	1:F:5319:ILE:HG13	2.00	0.44
1:F:5435:THR:OG1	1:F:5436:LEU:N	2.51	0.44
1:F:5451:PRO:HG3	1:F:5461:THR:OG1	2.18	0.44
1:G:6258:GLY:O	1:G:6261:ASN:N	2.50	0.44
1:G:6291:LEU:N	1:G:6291:LEU:HD23	2.33	0.44
1:G:6288:LEU:HG	1:G:6292:LEU:HG	2.00	0.44
1:H:7072:LEU:HG	1:H:7081:LYS:HD3	2.00	0.44
1:H:7094:LYS:O	1:H:7095:LEU:C	2.57	0.44
1:H:7168:GLY:O	1:H:7169:LEU:HD12	2.17	0.44
1:H:7288:LEU:O	1:H:7289:ALA:C	2.56	0.44
1:H:7292:LEU:O	1:H:7293:ALA:C	2.56	0.44
1:H:7292:LEU:O	1:H:7294:ALA:N	2.51	0.44
1:H:7421:ASN:HB2	3:H:7601:NAD:O2D	2.18	0.44
1:A:109:PRO:CA	1:A:113:THR:O	2.59	0.44
1:A:309:PHE:HB2	1:A:343:MSE:HG2	2.00	0.44
1:A:349:LEU:HD23	1:A:351:VAL:HB	2.00	0.44
1:A:389:ILE:HG22	1:A:415:VAL:O	2.18	0.44
1:A:421:ASN:HB3	1:A:422:PRO:HA	1.99	0.44
1:A:86:MSE:CE	1:A:86:MSE:HA	2.47	0.44
1:B:1397:ARG:HA	1:B:1427:GLU:O	2.18	0.44
1:C:2114:PRO:HD2	1:C:2115:THR:H	1.83	0.44
1:C:2240:LYS:HA	1:C:2243:THR:OG1	2.18	0.44
1:C:2328:VAL:C	1:C:2330:ASN:N	2.70	0.44
1:C:2569:VAL:O	1:C:2570:TYR:CB	2.66	0.44
1:D:3223:GLN:CG	1:D:3224:LYS:N	2.80	0.44
1:E:4268:LYS:HE2	1:E:4269:TYR:CE2	2.52	0.44
1:E:4332:LEU:HG	1:E:4336:GLU:OE2	2.18	0.44
1:F:5139:ASP:CG	1:F:5146:ILE:HD11	2.37	0.44
1:F:5356:ALA:C	1:F:5357:LYS:HD3	2.39	0.44
1:G:6026:LYS:N	1:G:6027:PRO:CD	2.81	0.44
1:G:6302:ILE:HA	1:G:6305:HIS:ND1	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:6300:LYS:O	1:G:6305:HIS:NE2	2.50	0.44
1:G:6377:PHE:O	1:G:6380:ALA:N	2.51	0.44
1:H:7104:ILE:HG13	1:H:7108:MSE:HE2	1.99	0.44
1:A:166:ILE:HD12	1:A:179:ILE:HG13	2.00	0.43
1:A:166:ILE:O	1:A:167:LEU:O	2.36	0.43
1:A:388:THR:HG23	1:A:415:VAL:CB	2.46	0.43
1:A:394:GLY:HA2	1:A:420:SER:CB	2.47	0.43
1:A:539:MSE:HB3	1:A:539:MSE:HE2	1.84	0.43
1:A:552:TYR:CE1	1:A:556:ARG:CZ	3.01	0.43
1:B:1048:LEU:HD22	1:B:1048:LEU:N	2.32	0.43
1:B:1054:LEU:O	1:B:1055:PRO:C	2.55	0.43
1:B:1090:GLU:HG2	1:B:1131:LYS:NZ	2.33	0.43
1:B:1338:GLN:HB3	1:B:1338:GLN:HE21	1.63	0.43
1:B:1336:GLU:O	1:B:1340:LYS:HG3	2.17	0.43
1:B:1524:ILE:O	1:B:1527:ALA:HB3	2.18	0.43
1:B:1555:GLU:O	1:B:1557:THR:N	2.50	0.43
1:C:2132:GLY:HA3	1:C:2177:MSE:HE2	1.99	0.43
1:C:2155:VAL:HB	1:C:2246:TYR:CD2	2.53	0.43
1:C:2388:THR:HA	1:C:2415:VAL:HG23	2.00	0.43
1:D:3108:MSE:HE2	1:D:3108:MSE:HB2	1.68	0.43
1:D:3259:ASN:N	1:D:3259:ASN:ND2	2.66	0.43
1:D:3269:TYR:O	1:D:3270:ARG:C	2.56	0.43
1:D:3094:LYS:HG2	1:D:3562:TYR:CD2	2.52	0.43
1:E:4381:VAL:HG13	1:E:4407:MSE:HE2	2.00	0.43
1:G:6296:LYS:O	1:G:6296:LYS:HG2	2.17	0.43
1:G:6335:GLN:HG3	1:G:6336:GLU:N	2.32	0.43
1:H:7089:GLN:O	1:H:7091:ARG:N	2.51	0.43
1:H:7309:PHE:HD2	1:H:7343:MSE:HG3	1.82	0.43
1:H:7324:VAL:HA	1:H:7327:MSE:CE	2.48	0.43
1:H:7338:GLN:HA	1:H:7341:ILE:HG13	2.00	0.43
1:A:258:GLY:O	1:A:261:ASN:N	2.51	0.43
1:A:333:SER:H	1:A:336:GLU:CD	2.22	0.43
1:A:359:ASP:O	1:A:363:GLU:HG2	2.19	0.43
1:A:458:ARG:NH1	1:A:458:ARG:HB2	2.33	0.43
1:A:471:PHE:CD1	1:A:472:PRO:CD	3.01	0.43
1:A:505:GLU:O	1:A:509:GLN:HG3	2.18	0.43
1:A:67:ARG:HA	1:B:1217:PHE:CE1	2.54	0.43
1:C:2543:TYR:CD2	1:C:2543:TYR:C	2.91	0.43
1:C:2553:VAL:O	1:C:2555:GLU:N	2.51	0.43
1:D:3045:ARG:HB3	1:D:3051:GLN:HG2	2.00	0.43
1:D:3259:ASN:O	1:D:3260:HIS:C	2.56	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:5036:LYS:O	1:F:5039:ALA:HB3	2.18	0.43
1:F:5083:ILE:HD11	1:F:5126:ILE:HB	1.99	0.43
1:F:5303:SER:N	1:F:5340:LYS:HZ1	2.15	0.43
1:F:5359:ASP:N	1:F:5362:GLN:OE1	2.51	0.43
1:F:5458:ARG:HH11	1:F:5458:ARG:HB2	1.81	0.43
1:G:6151:PRO:HG3	1:H:7026:LYS:HD3	2.00	0.43
1:G:6213:LEU:C	1:G:6214:LYS:HG3	2.36	0.43
1:G:6317:LEU:HA	1:G:6320:ALA:HB3	2.00	0.43
1:H:7079:LEU:O	1:H:7079:LEU:HG	2.17	0.43
1:H:7089:GLN:C	1:H:7091:ARG:H	2.21	0.43
1:H:7304:GLU:H	1:H:7304:GLU:CD	2.21	0.43
1:H:7523:SER:HA	1:H:7526:ILE:HG13	1.99	0.43
1:A:295:GLN:NE2	1:A:305:HIS:HE1	2.15	0.43
1:A:354:ARG:HE	1:A:356:ALA:HB3	1.83	0.43
1:A:385:LYS:N	1:A:386:PRO:CD	2.81	0.43
1:A:477:ALA:HB1	1:A:531:THR:HG22	1.99	0.43
1:B:1218:TYR:HB3	1:B:1222:TYR:CZ	2.53	0.43
1:B:1270:ARG:HG3	1:B:1271:GLU:N	2.33	0.43
1:B:1286:VAL:O	1:B:1289:ALA:HB3	2.17	0.43
1:B:1376:THR:CG2	1:B:1379:ASP:H	2.26	0.43
1:C:2376:THR:N	1:C:2379:ASP:HB2	2.28	0.43
1:D:3261:ASN:HA	1:D:3264:ARG:CG	2.47	0.43
1:D:3349:LEU:HD11	1:D:3384:LEU:HD21	2.00	0.43
1:D:3505:GLU:O	1:D:3509:GLN:HG3	2.18	0.43
1:D:3503:THR:OG1	1:D:3506:GLU:HG3	2.18	0.43
1:E:4068:PHE:HE2	1:E:4072:LEU:HD22	1.83	0.43
1:E:4333:SER:O	1:E:4334:GLU:C	2.56	0.43
1:F:5089:GLN:HB2	1:F:5096:PHE:CD1	2.52	0.43
1:F:5221:LEU:HB3	1:F:5223:GLN:NE2	2.33	0.43
1:F:5303:SER:O	1:F:5340:LYS:HE3	2.18	0.43
1:G:6077:SER:O	1:G:6081:LYS:HG3	2.19	0.43
1:G:6108:MSE:N	1:G:6109:PRO:CD	2.80	0.43
1:G:6300:LYS:HE3	1:G:6305:HIS:CD2	2.54	0.43
1:G:6494:ALA:O	1:G:6497:ALA:HB3	2.19	0.43
1:G:6506:GLU:HG3	1:G:6511:ARG:HD2	2.01	0.43
1:G:6094:LYS:HD2	1:G:6558:TRP:CZ2	2.53	0.43
1:H:7269:TYR:HB2	1:H:7275:THR:HG21	2.01	0.43
1:A:456:ASP:OD1	1:A:458:ARG:NH1	2.51	0.43
1:B:1541:PHE:CD2	1:B:1541:PHE:N	2.86	0.43
1:C:2184:LEU:O	1:C:2187:TYR:HB2	2.17	0.43
1:C:2232:ASP:HA	1:C:2235:ILE:HG12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3193:ILE:CG2	1:D:3194:ARG:N	2.81	0.43
1:E:4537:ASN:HB3	1:E:4539:MSE:CG	2.49	0.43
1:F:5227:ARG:NH1	1:F:5227:ARG:HG2	2.31	0.43
1:G:6205:VAL:HG21	1:G:6231:TYR:CE1	2.52	0.43
1:G:6385:LYS:HB2	1:G:6385:LYS:HE3	1.44	0.43
1:G:6413:ARG:NH2	1:G:6440:ARG:C	2.67	0.43
1:G:6535:TYR:CD1	1:G:6549:LYS:HE2	2.54	0.43
1:G:6130:PRO:HG2	1:H:7054:LEU:CD2	2.48	0.43
1:H:7066:LEU:HG	1:H:7070:ARG:HD3	1.99	0.43
1:H:7556:ARG:NE	3:H:7602:NAD:O2A	2.52	0.43
1:A:397:ARG:NH2	1:A:429:THR:CG2	2.78	0.43
1:A:453:LYS:HA	1:A:458:ARG:O	2.17	0.43
1:A:501:GLN:CA	1:A:501:GLN:NE2	2.79	0.43
1:B:1082:TYR:CZ	1:B:1086:MSE:HG3	2.53	0.43
1:B:1207:THR:N	1:B:1223:GLN:O	2.45	0.43
1:B:1276:PHE:CD1	1:B:1277:ASN:N	2.86	0.43
1:B:1319:ILE:O	1:B:1320:ALA:C	2.56	0.43
1:B:1346:LYS:HB3	3:B:1601:NAD:C4A	2.49	0.43
1:B:1417:PHE:HZ	1:B:1512:LEU:HD22	1.83	0.43
1:D:3266:LEU:O	1:D:3270:ARG:HB3	2.19	0.43
1:D:3324:VAL:HG21	1:D:3365:PHE:HZ	1.83	0.43
1:D:3327:MSE:HE3	1:D:3337:ALA:CA	2.49	0.43
1:E:4235:ILE:H	1:E:4235:ILE:HG12	1.70	0.43
1:E:4261:ASN:OD1	1:E:4264:ARG:NH2	2.52	0.43
1:E:4335:GLN:NE2	1:E:4339:LYS:HG3	2.34	0.43
1:E:4351:VAL:HG11	1:E:4369:ALA:HB2	2.01	0.43
1:E:4377:PHE:HZ	1:E:4389:ILE:HD11	1.83	0.43
1:F:5085:ILE:HG23	1:F:5086:MSE:CE	2.49	0.43
1:F:5521:GLU:CG	1:F:5522:VAL:N	2.81	0.43
1:G:6258:GLY:O	1:G:6259:ASN:C	2.57	0.43
1:H:7046:GLN:CG	1:H:7051:GLN:HG3	2.48	0.43
1:H:7351:VAL:HG21	1:H:7369:ALA:HA	2.00	0.43
1:H:7410:ILE:HG13	1:H:7410:ILE:H	1.58	0.43
1:H:7326:SER:HB2	1:H:7492:LEU:HD11	2.00	0.43
1:A:243:THR:O	1:A:247:GLY:N	2.38	0.43
1:A:301:PRO:O	1:A:304:GLU:HG3	2.19	0.43
1:A:306:LYS:H	1:A:387:SER:HB3	1.83	0.43
1:A:397:ARG:NH1	1:A:397:ARG:HG2	2.31	0.43
1:A:391:GLY:CA	1:A:427:GLU:HG2	2.45	0.43
1:B:1104:ILE:O	1:B:1108:MSE:HB2	2.18	0.43
1:B:1159:VAL:CG1	1:B:1180:PRO:HB3	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1319:ILE:H	1:B:1319:ILE:HG13	1.56	0.43
1:B:1495:ALA:O	1:B:1496:LYS:C	2.55	0.43
1:C:2023:GLU:N	4:C:8045:HOH:O	2.50	0.43
1:C:2244:ASP:N	1:C:2248:ARG:HH12	2.15	0.43
1:C:2298:ILE:HG22	1:C:2299:SER:N	2.32	0.43
1:C:2300:LYS:NZ	1:C:2305:HIS:HD2	2.16	0.43
1:D:3075:MSE:HB2	1:D:3075:MSE:HE3	1.71	0.43
1:D:3136:SER:O	1:D:3139:ASP:HB2	2.18	0.43
1:D:3333:SER:HB3	1:D:3336:GLU:HG3	1.99	0.43
1:E:4023:GLU:OE1	1:E:4023:GLU:HA	2.19	0.43
1:E:4048:LEU:HD22	1:E:4048:LEU:N	2.34	0.43
1:E:4155:VAL:HG21	1:E:4246:TYR:CZ	2.53	0.43
1:F:5030:LEU:N	1:F:5030:LEU:HD23	2.34	0.43
1:F:5504:ASP:O	1:F:5507:LEU:HB2	2.18	0.43
1:G:6040:PHE:O	1:G:6045:ARG:NE	2.52	0.43
1:G:6137:ILE:HA	1:G:6234:LEU:HD21	1.99	0.43
1:G:6208:ASP:OD2	1:G:6227:ARG:NH2	2.43	0.43
1:G:6302:ILE:HG22	1:G:6340:LYS:HZ3	1.83	0.43
1:G:6300:LYS:HE3	1:G:6305:HIS:HD2	1.84	0.43
1:G:6308:LEU:HD22	1:G:6384:LEU:HD23	2.01	0.43
1:G:6482:ASN:ND2	1:G:6482:ASN:N	2.63	0.43
1:H:7277:ASN:OD1	1:H:7277:ASN:C	2.57	0.43
1:H:7276:PHE:CB	1:H:7281:GLN:OE1	2.60	0.43
1:H:7493:GLU:HA	1:H:7496:LYS:HD3	2.01	0.43
1:A:308:LEU:HB3	1:A:389:ILE:HD13	2.00	0.43
1:A:429:THR:HG23	1:A:432:GLU:CD	2.39	0.43
1:B:1071:ASN:HA	1:B:1074:LYS:HE3	2.00	0.43
1:A:57:LYS:HB2	1:B:1219:MSE:C	2.39	0.43
1:B:1288:LEU:HD11	1:B:1323:ILE:HA	2.00	0.43
1:B:1453:LYS:CB	1:B:1459:VAL:HG13	2.48	0.43
1:B:1454:LEU:HD13	1:B:1458:ARG:NH1	2.34	0.43
1:C:2297:VAL:HG23	1:C:2298:ILE:HD13	1.99	0.43
1:C:2385:LYS:HE2	1:C:2385:LYS:HB2	1.57	0.43
1:C:2309:PHE:CD1	1:C:2390:ILE:HB	2.53	0.43
1:C:2432:GLU:C	1:C:2436:LEU:HD13	2.38	0.43
1:D:3174:VAL:HG22	1:D:3218:TYR:CE2	2.54	0.43
1:E:4031:ASN:HA	1:E:4032:PRO:HD2	1.75	0.43
1:E:4176:GLY:O	1:E:4177:MSE:C	2.56	0.43
1:E:4548:ASP:OD1	1:E:4550:ALA:HB3	2.19	0.43
1:F:5024:LYS:HA	1:F:5028:LEU:HD22	2.00	0.43
1:F:5252:ILE:O	1:F:5275:THR:HA	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:6166:ILE:HA	1:G:6256:ASP:CG	2.38	0.43
1:G:6468:VAL:HG22	1:G:6468:VAL:O	2.18	0.43
1:H:7210:ILE:HD13	1:H:7210:ILE:N	2.33	0.43
1:H:7255:GLU:O	1:H:7257:PHE:HD1	2.00	0.43
1:A:335:GLN:HE21	1:A:339:LYS:CG	2.31	0.43
1:A:529:LYS:HD2	1:A:529:LYS:HA	1.84	0.43
1:A:59:GLU:HG2	1:A:63:ILE:CG2	2.41	0.43
1:A:30:LEU:HB3	1:B:1030:LEU:HD13	2.01	0.43
1:B:1184:LEU:HA	1:B:1184:LEU:HD12	1.90	0.43
1:B:1239:MSE:HE2	1:B:1273:TYR:CD1	2.54	0.43
1:B:1315:ALA:HB1	1:B:1319:ILE:HD11	2.00	0.43
1:B:1298:ILE:CD1	1:B:1413:ARG:HD3	2.49	0.43
1:C:2090:GLU:CG	1:C:2131:LYS:HD3	2.48	0.43
1:C:2177:MSE:CE	1:C:2200:PRO:HB2	2.49	0.43
1:C:2260:HIS:CE1	1:C:2264:ARG:NE	2.86	0.43
1:C:2370:PRO:O	1:C:2371:GLU:C	2.56	0.43
1:C:2453:LYS:NZ	1:C:2457:GLY:HA2	2.33	0.43
1:D:3416:ILE:N	1:D:3416:ILE:HD13	2.34	0.43
1:D:3416:ILE:HD12	1:D:3441:CYS:HB2	2.00	0.43
1:E:4363:GLU:O	1:E:4365:PHE:N	2.51	0.43
1:F:5085:ILE:O	1:F:5088:ILE:HG12	2.19	0.43
1:F:5210:ILE:N	1:F:5210:ILE:HD13	2.34	0.43
1:G:6224:LYS:HD2	1:G:6224:LYS:HA	1.73	0.43
1:H:7026:LYS:HA	1:H:7029:MSE:HE2	2.00	0.43
1:H:7047:MSE:O	1:H:7048:LEU:HD22	2.19	0.43
1:H:7469:TYR:HA	1:H:7519:ILE:HD11	2.00	0.43
1:A:146:ILE:CD1	1:A:146:ILE:N	2.78	0.43
1:A:219:MSE:CG	1:A:219:MSE:O	2.65	0.43
1:A:395:ALA:O	1:A:398:LEU:HD11	2.19	0.43
1:A:559:ARG:HD3	1:A:559:ARG:HA	1.72	0.43
1:B:1170:GLY:O	1:B:1171:ASP:C	2.57	0.43
1:B:1194:ARG:HG3	3:B:1602:NAD:C6A	2.48	0.43
1:B:1164:GLU:OE1	1:B:1225:ARG:NH1	2.52	0.43
1:B:1315:ALA:O	1:B:1319:ILE:HG13	2.19	0.43
1:C:2103:ASP:HB3	1:C:2107:LEU:CD2	2.49	0.43
1:C:2309:PHE:CE1	1:C:2390:ILE:CD1	3.02	0.43
1:C:2400:THR:OG1	1:C:2402:ASP:HB2	2.19	0.43
1:D:3112:TYR:HA	1:D:3116:VAL:HB	2.01	0.43
1:D:3337:ALA:C	1:D:3339:LYS:N	2.71	0.43
1:D:3369:ALA:HA	1:D:3370:PRO:HD3	1.89	0.43
1:D:3289:ALA:CB	1:D:3498:LEU:HD23	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:4344:PHE:HA	1:E:4349:LEU:HA	2.01	0.43
1:F:5277:ASN:C	1:F:5277:ASN:OD1	2.57	0.43
1:F:5338:GLN:O	1:F:5367:HIS:CE1	2.72	0.43
1:G:6116:VAL:HG13	1:G:6117:GLY:N	2.34	0.43
1:G:6227:ARG:NH1	1:G:6227:ARG:CG	2.82	0.43
1:G:6231:TYR:O	1:G:6235:ILE:HG12	2.18	0.43
1:G:6342:TRP:CE3	1:G:6349:LEU:HD21	2.52	0.43
1:G:6437:THR:C	1:G:6439:GLY:N	2.69	0.43
1:H:7384:LEU:O	1:H:7385:LYS:HB2	2.18	0.43
1:A:104:ILE:HG23	1:A:105:GLU:H	1.83	0.43
1:A:407:MSE:HA	1:A:410:ILE:HD12	2.01	0.43
1:A:411:ASN:O	1:A:440:ARG:NH1	2.43	0.43
1:A:472:PRO:O	1:A:475:ALA:HB3	2.18	0.43
1:B:1150:TRP:CD1	1:B:1152:GLU:HB2	2.54	0.43
1:B:1288:LEU:O	1:B:1292:LEU:HG	2.18	0.43
1:B:1421:ASN:N	3:B:1601:NAD:O2D	2.52	0.43
1:C:2089:GLN:HB2	1:C:2096:PHE:CD1	2.53	0.43
1:C:2283:THR:O	1:C:2284:ALA:C	2.57	0.43
1:C:2308:LEU:HD13	1:C:2342:TRP:HB3	1.99	0.43
1:C:2383:ILE:HG12	1:C:2383:ILE:H	1.53	0.43
1:C:2414:PRO:HD2	1:C:2441:CYS:CA	2.47	0.43
1:C:2451:PRO:HA	1:C:2462:PRO:HD3	2.00	0.43
1:C:2482:ASN:N	1:C:2482:ASN:ND2	2.67	0.43
1:D:3302:ILE:HD11	1:D:3330:ASN:HD22	1.84	0.43
1:D:3397:ARG:NH2	1:D:3429:THR:HG22	2.34	0.43
1:D:3290:GLY:HA3	1:D:3417:PHE:CE2	2.54	0.43
1:E:4082:TYR:HD1	1:E:4110:ILE:O	2.02	0.43
1:E:4309:PHE:HB2	1:E:4343:MSE:CG	2.49	0.43
1:F:5278:ASP:C	1:F:5280:ILE:H	2.22	0.43
1:F:5437:THR:O	1:F:5440:ARG:N	2.52	0.43
1:G:6068:PHE:CZ	1:G:6072:LEU:HD13	2.54	0.43
1:G:6399:PHE:CG	1:G:6427:GLU:HB3	2.54	0.43
1:G:6466:ASN:ND2	1:G:6468:VAL:HG12	2.34	0.43
1:G:6130:PRO:HG2	1:H:7054:LEU:HD23	2.00	0.43
1:H:7085:ILE:O	1:H:7087:GLY:N	2.52	0.43
1:H:7274:CYS:SG	1:H:7486:ILE:HD11	2.59	0.43
1:H:7343:MSE:CB	1:H:7350:LEU:HD23	2.41	0.43
1:H:7359:ASP:N	1:H:7362:GLN:OE1	2.50	0.43
1:H:7511:ARG:NH1	1:H:7513:TYR:O	2.52	0.43
1:H:7527:ALA:O	1:H:7528:ILE:C	2.57	0.43
1:A:156:LYS:HA	1:A:156:LYS:HE2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:TYR:O	1:A:175:TYR:CE1	2.71	0.42
1:A:217:PHE:CZ	1:B:1066:LEU:HG	2.53	0.42
1:A:174:VAL:HG22	1:A:218:TYR:CE2	2.54	0.42
1:A:338:GLN:C	1:A:340:LYS:H	2.22	0.42
1:A:400:THR:HG23	1:A:403:VAL:HB	2.00	0.42
1:A:396:GLY:N	1:A:425:GLN:O	2.51	0.42
1:C:2176:GLY:O	1:C:2178:GLY:N	2.52	0.42
1:C:2232:ASP:O	1:C:2233:ASP:C	2.58	0.42
1:C:2240:LYS:O	1:C:2244:ASP:HB2	2.19	0.42
1:D:3248:ARG:HD2	1:D:3248:ARG:HA	1.74	0.42
1:D:3267:ARG:HH11	1:D:3267:ARG:CG	2.31	0.42
1:D:3484:ARG:C	1:D:3485:HIS:ND1	2.72	0.42
1:D:3558:TRP:CG	1:D:3559:ARG:N	2.86	0.42
1:E:4358:ILE:HG21	1:E:4366:THR:HG21	2.00	0.42
1:E:4378:GLU:O	1:E:4381:VAL:HB	2.18	0.42
1:F:5332:LEU:HD22	1:F:5337:ALA:HA	2.01	0.42
1:F:5506:GLU:CG	1:F:5511:ARG:HD2	2.44	0.42
1:G:6120:CYS:O	1:G:6123:TYR:HB2	2.18	0.42
1:G:6122:GLN:C	1:G:6126:ILE:HG12	2.38	0.42
1:G:6271:GLU:HA	1:G:6485:HIS:CD2	2.54	0.42
1:G:6321:ASN:O	1:G:6324:VAL:HB	2.19	0.42
1:G:6342:TRP:CZ2	1:G:6384:LEU:HD11	2.54	0.42
1:H:7333:SER:O	1:H:7334:GLU:C	2.57	0.42
1:H:7566:LEU:HA	1:H:7566:LEU:HD23	1.79	0.42
1:A:251:LEU:HA	1:A:274:CYS:O	2.19	0.42
1:A:43:GLN:CG	1:A:47:MSE:HE3	2.49	0.42
1:A:551:LYS:O	1:A:555:GLU:HB2	2.19	0.42
1:C:2023:GLU:HA	1:C:2023:GLU:OE1	2.19	0.42
1:C:2338:GLN:HB3	1:C:2338:GLN:HE21	1.54	0.42
1:C:2345:ASP:HB2	3:C:2601:NAD:O2B	2.19	0.42
1:C:2527:ALA:O	1:C:2528:ILE:C	2.57	0.42
1:D:3081:LYS:O	1:D:3085:ILE:HG22	2.19	0.42
1:D:3155:VAL:H	1:D:3246:TYR:HD2	1.66	0.42
1:E:4211:ALA:HA	1:E:4214:LYS:HD3	2.01	0.42
1:E:4261:ASN:ND2	1:E:4261:ASN:N	2.50	0.42
1:E:4410:ILE:HG13	1:E:4410:ILE:H	1.55	0.42
1:E:4389:ILE:HG22	1:E:4416:ILE:HG22	2.01	0.42
1:F:5310:LEU:HG	1:F:5393:ALA:CB	2.43	0.42
1:F:5400:THR:CB	1:F:5401:PRO:HD2	2.48	0.42
1:F:5485:HIS:ND1	1:F:5485:HIS:N	2.67	0.42
1:G:6243:THR:C	1:G:6248:ARG:HH11	2.23	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:6255:GLU:HB3	1:G:6256:ASP:H	1.62	0.42
1:H:7288:LEU:O	1:H:7290:GLY:N	2.51	0.42
1:A:425:GLN:N	1:A:425:GLN:HE21	2.17	0.42
1:A:499:THR:O	1:A:501:GLN:N	2.51	0.42
1:B:1347:TYR:HB2	1:B:1354:ARG:HH22	1.84	0.42
1:C:2126:ILE:O	1:C:2128:ARG:HD3	2.19	0.42
1:C:2293:ALA:O	1:C:2297:VAL:HG13	2.19	0.42
1:C:2285:ALA:HB1	1:C:2470:ILE:HG13	2.01	0.42
1:C:2498:LEU:O	1:C:2501:GLN:CB	2.66	0.42
1:C:2480:LEU:HD21	1:C:2556:ARG:HB3	2.00	0.42
1:D:3324:VAL:HG21	1:D:3365:PHE:CZ	2.55	0.42
1:D:3367:HIS:ND1	1:D:3367:HIS:N	2.67	0.42
1:D:3400:THR:HG23	1:D:3403:VAL:CG2	2.48	0.42
1:E:4293:ALA:O	1:E:4296:LYS:CB	2.67	0.42
1:E:4304:GLU:H	1:E:4304:GLU:HG3	1.31	0.42
1:E:4401:PRO:O	1:E:4405:ARG:N	2.47	0.42
1:E:4506:GLU:HG2	1:E:4511:ARG:CD	2.49	0.42
1:F:5026:LYS:C	1:F:5028:LEU:N	2.73	0.42
1:G:6122:GLN:O	1:G:6125:HIS:CB	2.68	0.42
1:G:6137:ILE:HG22	1:G:6221:LEU:HD21	2.01	0.42
1:G:6394:GLY:CA	1:G:6425:GLN:HG3	2.49	0.42
1:H:7202:CYS:SG	1:H:7203:ILE:N	2.92	0.42
1:H:7270:ARG:CG	1:H:7271:GLU:N	2.80	0.42
1:H:7359:ASP:C	1:H:7359:ASP:OD2	2.57	0.42
1:H:7534:LEU:HA	1:H:7539:MSE:HG3	2.00	0.42
1:A:193:ILE:O	1:A:195:PRO:HD3	2.19	0.42
1:A:454:LEU:HD13	1:A:458:ARG:HH12	1.77	0.42
1:B:1069:HIS:O	1:B:1071:ASN:N	2.53	0.42
1:B:1085:ILE:HG23	1:B:1086:MSE:CE	2.49	0.42
1:B:1144:ARG:HH12	1:B:1245:ARG:N	2.16	0.42
1:A:57:LYS:HB2	1:B:1219:MSE:HA	2.01	0.42
1:C:2048:LEU:HD22	1:C:2048:LEU:N	2.33	0.42
1:C:2232:ASP:O	1:C:2235:ILE:N	2.52	0.42
1:C:2425:GLN:O	1:C:2426:ALA:O	2.36	0.42
1:C:2494:ALA:O	1:C:2497:ALA:HB3	2.18	0.42
1:D:3137:ILE:O	1:D:3139:ASP:N	2.51	0.42
1:D:3208:ASP:O	1:D:3210:ILE:HD13	2.19	0.42
1:D:3238:PHE:CD2	1:D:3239:MSE:HG2	2.54	0.42
1:D:3255:GLU:O	1:D:3257:PHE:N	2.53	0.42
1:D:3261:ASN:O	1:D:3264:ARG:HG2	2.19	0.42
1:D:3486:ILE:H	1:D:3486:ILE:HG12	1.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:4310:LEU:HD23	1:E:4427:GLU:CG	2.49	0.42
1:F:5243:THR:HA	1:F:5247:GLY:O	2.19	0.42
1:F:5295:GLN:HE22	1:F:5305:HIS:CE1	2.38	0.42
1:F:5487:SER:O	1:F:5490:VAL:CG2	2.61	0.42
1:G:6069:HIS:C	1:G:6071:ASN:H	2.22	0.42
1:G:6177:MSE:O	1:G:6177:MSE:HE3	2.19	0.42
1:G:6188:THR:HG23	1:G:6193:ILE:O	2.20	0.42
1:G:6306:LYS:O	1:G:6386:PRO:HA	2.19	0.42
1:H:7571:GLU:HG3	1:H:7571:GLU:O	2.20	0.42
1:A:127:PHE:CD2	1:A:127:PHE:C	2.92	0.42
1:A:324:VAL:HG12	1:A:325:MSE:N	2.33	0.42
1:A:298:ILE:HD12	1:A:413:ARG:HD3	2.00	0.42
1:B:1137:ILE:N	1:B:1204:ASP:O	2.49	0.42
1:C:2154:HIS:HB3	1:C:2197:ARG:HD2	2.02	0.42
1:C:2278:ASP:C	1:C:2280:ILE:N	2.73	0.42
1:C:2376:THR:O	1:C:2377:PHE:C	2.57	0.42
1:C:2416:ILE:CD1	1:C:2416:ILE:H	2.23	0.42
1:C:2528:ILE:HD13	1:C:2553:VAL:HB	2.00	0.42
1:D:3122:GLN:O	1:D:3123:TYR:C	2.57	0.42
1:D:3182:GLY:O	1:D:3185:CYS:HB2	2.20	0.42
1:D:3507:LEU:HA	1:D:3507:LEU:HD13	1.83	0.42
1:E:4068:PHE:CD2	1:E:4068:PHE:C	2.92	0.42
1:E:4388:THR:HA	1:E:4415:VAL:HB	2.02	0.42
1:E:4419:LEU:N	1:E:4419:LEU:HD13	2.34	0.42
1:E:4549:LYS:N	1:E:4549:LYS:HD3	2.35	0.42
1:F:5116:VAL:HG13	1:F:5117:GLY:N	2.34	0.42
1:F:5271:GLU:O	1:F:5485:HIS:NE2	2.53	0.42
1:F:5303:SER:C	1:F:5340:LYS:HE3	2.40	0.42
1:F:5358:ILE:HD12	1:F:5358:ILE:N	2.34	0.42
1:F:5416:ILE:H	1:F:5416:ILE:CD1	2.29	0.42
1:G:6026:LYS:HB3	1:G:6027:PRO:HD3	2.00	0.42
1:G:6194:ARG:HB2	1:G:6197:ARG:CG	2.42	0.42
1:G:6210:ILE:HA	1:G:6213:LEU:HB2	2.01	0.42
1:G:6276:PHE:HD1	1:G:6277:ASN:N	2.17	0.42
1:G:6351:VAL:HA	1:G:6367:HIS:O	2.20	0.42
1:H:7325:MSE:HB3	1:H:7325:MSE:HE2	1.95	0.42
1:H:7553:VAL:O	1:H:7556:ARG:N	2.47	0.42
1:A:215:ASP:HB3	1:A:218:TYR:HB2	2.01	0.42
1:A:270:ARG:HG3	1:A:271:GLU:N	2.34	0.42
1:A:325:MSE:HE2	1:A:492:LEU:CD1	2.46	0.42
1:A:397:ARG:HH22	1:A:429:THR:HG22	1.80	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:566:LEU:HA	1:A:566:LEU:HD23	1.75	0.42
1:B:1359:ASP:OD2	1:B:1362:GLN:CB	2.68	0.42
1:B:1376:THR:N	1:B:1379:ASP:HB2	2.35	0.42
1:C:2094:LYS:HD3	1:C:2558:TRP:HZ2	1.84	0.42
1:C:2169:LEU:N	1:C:2169:LEU:CD1	2.82	0.42
1:C:2382:ASN:O	1:C:2384:LEU:N	2.53	0.42
1:C:2431:GLU:C	1:C:2433:ALA:N	2.72	0.42
1:D:3036:LYS:O	1:D:3037:GLY:C	2.55	0.42
1:D:3072:LEU:HG	1:D:3081:LYS:HD2	2.01	0.42
1:D:3082:TYR:HB2	1:D:3110:ILE:HG23	2.00	0.42
1:D:3082:TYR:O	1:D:3085:ILE:CG2	2.66	0.42
1:D:3144:ARG:O	1:D:3147:VAL:HB	2.20	0.42
1:D:3415:VAL:HG13	1:D:3442:LEU:HB2	2.02	0.42
1:D:3491:PHE:O	1:D:3492:LEU:C	2.57	0.42
1:D:3417:PHE:CZ	1:D:3512:LEU:HD22	2.53	0.42
1:E:4089:GLN:C	1:E:4091:ARG:H	2.23	0.42
1:E:4122:GLN:O	1:E:4123:TYR:C	2.58	0.42
1:E:4209:ASN:HB3	1:E:4212:LEU:HD12	2.01	0.42
1:E:4218:TYR:O	1:F:5057:LYS:CE	2.67	0.42
1:E:4359:ASP:HB3	1:E:4362:GLN:OE1	2.20	0.42
1:F:5376:THR:CG2	1:F:5378:GLU:H	2.29	0.42
1:F:5397:ARG:C	1:F:5398:LEU:HD12	2.40	0.42
1:G:6079:LEU:HD11	1:G:6119:ALA:CA	2.49	0.42
1:G:6116:VAL:O	1:G:6120:CYS:N	2.48	0.42
1:G:6123:TYR:C	1:G:6125:HIS:N	2.69	0.42
1:G:6300:LYS:CD	1:G:6304:GLU:HB2	2.48	0.42
1:G:6402:ASP:O	1:G:6405:ARG:HG2	2.20	0.42
1:G:6429:THR:HG23	1:G:6432:GLU:CG	2.50	0.42
1:A:244:ASP:OD1	1:A:248:ARG:NH1	2.53	0.42
1:A:376:THR:CG2	1:A:377:PHE:N	2.82	0.42
1:A:546:PRO:HG2	1:A:549:LYS:HD2	2.00	0.42
1:A:57:LYS:HG3	1:B:1219:MSE:HA	2.00	0.42
1:B:1101:GLN:HG3	1:B:1101:GLN:H	1.54	0.42
1:B:1122:GLN:O	1:B:1125:HIS:HB2	2.19	0.42
1:B:1412:GLU:O	1:B:1440:ARG:NH1	2.49	0.42
1:B:1422:PRO:HB2	1:B:1423:THR:H	1.72	0.42
1:C:2072:LEU:HD11	1:C:2081:LYS:CB	2.47	0.42
1:C:2218:TYR:CD2	1:C:2219:MSE:N	2.88	0.42
1:C:2244:ASP:HA	1:C:2248:ARG:NH1	2.34	0.42
1:C:2470:ILE:C	1:C:2472:PRO:CD	2.88	0.42
1:C:2482:ASN:N	1:C:2482:ASN:HD22	2.17	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3119:ALA:O	1:D:3122:GLN:N	2.53	0.42
1:E:4068:PHE:CE1	1:E:4084:TYR:CE2	3.07	0.42
1:E:4416:ILE:O	1:E:4416:ILE:HG12	2.20	0.42
1:E:4397:ARG:NH1	1:E:4429:THR:HG22	2.34	0.42
1:F:5294:ALA:O	1:F:5297:VAL:HG22	2.19	0.42
1:F:5453:LYS:HB2	1:F:5459:VAL:CG1	2.29	0.42
1:F:5467:ASN:O	1:F:5469:TYR:N	2.52	0.42
1:F:5520:GLN:O	1:F:5523:SER:HB2	2.19	0.42
1:G:6100:LEU:CD2	1:G:6189:ALA:HB2	2.48	0.42
1:H:7386:PRO:HG2	1:H:7407:MSE:SE	2.69	0.42
1:H:7471:PHE:CE1	1:H:7472:PRO:HG3	2.54	0.42
1:H:7550:ALA:O	1:H:7554:LYS:CG	2.64	0.42
1:A:235:ILE:O	1:A:239:MSE:HG2	2.20	0.42
1:A:258:GLY:O	1:A:260:HIS:N	2.53	0.42
1:A:277:ASN:OD1	1:A:280:ILE:HG13	2.19	0.42
1:A:307:ILE:HG13	1:A:388:THR:OG1	2.19	0.42
1:A:440:ARG:HB3	1:A:440:ARG:CZ	2.49	0.42
1:B:1169:LEU:HD12	1:B:1169:LEU:N	2.34	0.42
1:B:1243:THR:HB	1:B:1248:ARG:NH1	2.34	0.42
1:B:1335:GLN:HA	1:B:1338:GLN:OE1	2.19	0.42
1:C:2266:LEU:HD12	1:C:2270:ARG:HB3	2.02	0.42
1:C:2332:LEU:HG	1:C:2336:GLU:OE2	2.20	0.42
1:C:2413:ARG:HH21	1:C:2440:ARG:C	2.23	0.42
1:D:3166:ILE:HG21	1:D:3172:LEU:CD1	2.46	0.42
1:D:3174:VAL:CG1	1:D:3220:GLY:HA3	2.49	0.42
1:D:3144:ARG:HH12	1:D:3244:ASP:C	2.23	0.42
1:D:3480:LEU:HD21	1:D:3556:ARG:CB	2.50	0.42
1:F:5086:MSE:HE3	1:F:5111:VAL:HG22	2.02	0.42
1:F:5331:GLY:O	1:F:5332:LEU:O	2.37	0.42
1:G:6175:TYR:CE2	1:G:6218:TYR:HD2	2.38	0.42
1:H:7359:ASP:O	1:H:7362:GLN:HB2	2.20	0.42
1:H:7388:THR:OG1	1:H:7415:VAL:CG2	2.68	0.42
1:H:7410:ILE:HB	1:H:7411:ASN:ND2	2.35	0.42
1:H:7521:GLU:HG3	1:H:7522:VAL:N	2.35	0.42
1:A:171:ASP:C	1:A:171:ASP:OD1	2.57	0.42
1:A:247:GLY:O	1:A:250:THR:HG22	2.20	0.42
1:A:415:VAL:HG12	1:A:417:PHE:HE1	1.85	0.42
1:B:1164:GLU:CD	1:B:1225:ARG:HD3	2.39	0.42
1:B:1351:VAL:C	1:B:1366:THR:HG22	2.40	0.42
1:B:1407:MSE:HG3	1:B:1414:PRO:HB3	2.02	0.42
1:C:2522:VAL:HG12	1:C:2526:ILE:HD11	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3088:ILE:HD13	1:D:3088:ILE:N	2.35	0.42
1:D:3321:ASN:O	1:D:3324:VAL:N	2.53	0.42
1:D:3571:GLU:O	1:D:3571:GLU:HG3	2.20	0.42
1:E:4253:GLN:HG3	1:E:4276:PHE:CE2	2.54	0.42
1:E:4431:GLU:O	1:E:4435:THR:HG23	2.19	0.42
1:F:5137:ILE:CG2	1:F:5138:SER:N	2.82	0.42
1:F:5432:GLU:HG2	1:F:5432:GLU:H	1.62	0.42
1:F:5451:PRO:HA	1:F:5462:PRO:HD2	2.01	0.42
1:F:5466:ASN:CB	1:F:5468:VAL:HG12	2.46	0.42
1:F:5570:TYR:CZ	1:H:7046:GLN:NE2	2.81	0.42
1:G:6146:ILE:O	1:G:6147:VAL:C	2.57	0.42
1:G:6199:LEU:HD12	1:G:6200:PRO:HD2	2.02	0.42
1:G:6165:ARG:NE	1:G:6259:ASN:ND2	2.67	0.42
1:G:6358:ILE:HG12	1:G:6366:THR:HG21	2.01	0.42
1:H:7132:GLY:HA3	1:H:7177:MSE:HE2	2.01	0.42
1:H:7161:THR:OG1	1:H:7162:ASP:N	2.53	0.42
1:H:7159:VAL:HG21	1:H:7184:LEU:HD13	2.01	0.42
1:H:7416:ILE:CD1	1:H:7416:ILE:N	2.83	0.42
1:H:7542:ARG:HD3	1:H:7543:TYR:N	2.33	0.42
1:A:320:ALA:HB1	1:A:365:PHE:CZ	2.54	0.42
1:A:335:GLN:HG3	1:A:336:GLU:N	2.34	0.42
1:A:416:ILE:HG12	1:A:416:ILE:O	2.19	0.42
1:B:1302:ILE:O	1:B:1303:SER:C	2.58	0.42
1:B:1345:ASP:HB2	3:B:1601:NAD:O2B	2.19	0.42
1:B:1453:LYS:HB2	1:B:1459:VAL:HG13	2.00	0.42
1:C:2269:TYR:O	1:C:2270:ARG:C	2.56	0.42
1:C:2398:LEU:N	1:C:2398:LEU:CD1	2.80	0.42
1:C:2401:PRO:HA	1:C:2436:LEU:CD2	2.50	0.42
1:C:2399:PHE:CB	1:C:2428:CYS:HB3	2.48	0.42
1:C:2416:ILE:CD1	1:C:2442:LEU:O	2.63	0.42
1:C:2518:ASN:O	1:C:2522:VAL:HG23	2.19	0.42
1:C:2552:TYR:CE1	1:C:2556:ARG:CZ	3.02	0.42
1:C:2129:ARG:NH2	1:D:3129:ARG:NH2	2.67	0.42
1:D:3496:LYS:O	1:D:3497:ALA:C	2.57	0.42
1:E:4070:ARG:O	1:E:4073:LYS:HB3	2.19	0.42
1:F:5254:PHE:HD2	1:F:5257:PHE:CE1	2.37	0.42
1:F:5401:PRO:O	1:F:5405:ARG:N	2.44	0.42
1:G:6038:MSE:HE2	1:G:6038:MSE:HB3	2.01	0.42
1:G:6191:ALA:HB1	1:G:6476:LEU:HD23	2.00	0.42
1:G:6238:PHE:HA	1:G:6241:ALA:HB3	2.02	0.42
1:H:7033:ARG:NH1	1:H:7152:GLU:OE1	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:7242:ILE:HG22	1:H:7243:THR:N	2.35	0.42
1:H:7298:ILE:HD11	1:H:7442:LEU:CD2	2.49	0.42
1:A:183:LYS:NZ	1:A:255:GLU:OE2	2.52	0.41
1:A:275:THR:O	1:A:486:ILE:HG13	2.20	0.41
1:A:521:GLU:CG	1:A:522:VAL:N	2.83	0.41
1:B:1044:GLU:O	1:B:1048:LEU:HB2	2.20	0.41
1:B:1162:ASP:OD2	1:B:1225:ARG:NH1	2.53	0.41
1:B:1194:ARG:HB2	1:B:1197:ARG:HG3	2.02	0.41
1:B:1321:ASN:O	1:B:1322:LEU:C	2.58	0.41
1:C:2376:THR:O	1:C:2379:ASP:N	2.53	0.41
1:D:3306:LYS:O	1:D:3386:PRO:HA	2.20	0.41
1:D:3474:VAL:O	1:D:3475:ALA:C	2.58	0.41
1:E:4104:ILE:O	1:E:4108:MSE:HE2	2.20	0.41
1:E:4120:CYS:O	1:E:4175:TYR:HB3	2.20	0.41
1:E:4179:ILE:O	1:E:4180:PRO:C	2.58	0.41
1:E:4312:ALA:HB2	1:E:4343:MSE:HE3	1.97	0.41
1:E:4351:VAL:CG1	1:E:4352:LYS:N	2.82	0.41
1:F:5219:MSE:HE3	1:F:5219:MSE:HB2	1.95	0.41
1:F:5254:PHE:CD2	1:F:5257:PHE:CE1	3.08	0.41
1:G:6060:THR:O	1:G:6062:ASP:N	2.53	0.41
1:G:6535:TYR:HA	1:G:6540:ALA:HB3	2.02	0.41
1:H:7075:MSE:HG3	1:H:7080:GLU:OE1	2.20	0.41
1:H:7271:GLU:HA	1:H:7485:HIS:HD2	1.85	0.41
1:H:7281:GLN:HB2	1:H:7491:PHE:CE2	2.55	0.41
1:B:1026:LYS:N	1:B:1027:PRO:CD	2.83	0.41
1:B:1081:LYS:O	1:B:1082:TYR:C	2.58	0.41
1:B:1144:ARG:O	1:B:1148:ASP:CG	2.59	0.41
1:B:1289:ALA:O	1:B:1499:THR:OG1	2.37	0.41
1:B:1291:LEU:HD23	1:B:1417:PHE:CE2	2.55	0.41
1:B:1341:ILE:HD12	1:B:1365:PHE:HE2	1.85	0.41
1:C:2175:TYR:CD1	1:C:2212:LEU:HD21	2.55	0.41
1:C:2344:PHE:CD1	1:C:2349:LEU:HA	2.55	0.41
1:D:3133:LEU:HD23	1:D:3199:LEU:HD11	2.02	0.41
1:D:3333:SER:CB	1:D:3336:GLU:HG3	2.49	0.41
1:D:3407:MSE:SE	1:D:3411:ASN:HD21	2.52	0.41
1:E:4094:LYS:O	1:E:4095:LEU:C	2.59	0.41
1:E:4116:VAL:CG1	1:E:4117:GLY:N	2.84	0.41
1:E:4313:GLY:HA3	3:E:4601:NAD:O5B	2.20	0.41
1:E:4334:GLU:O	1:E:4338:GLN:OE1	2.38	0.41
1:E:4336:GLU:O	1:E:4340:LYS:HG3	2.20	0.41
1:E:4453:LYS:HD3	1:E:4457:GLY:CA	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:5309:PHE:HD2	1:F:5343:MSE:HG2	1.86	0.41
1:F:5335:GLN:HA	1:F:5335:GLN:NE2	2.35	0.41
1:F:5420:SER:HB2	1:F:5426:ALA:HA	2.02	0.41
1:F:5533:TYR:CD2	1:F:5534:LEU:N	2.88	0.41
1:G:6298:ILE:HG22	1:G:6300:LYS:N	2.35	0.41
1:G:6300:LYS:HD2	1:G:6304:GLU:CG	2.50	0.41
1:G:6351:VAL:C	1:G:6366:THR:HG22	2.41	0.41
1:G:6377:PHE:CZ	1:G:6389:ILE:HD11	2.56	0.41
1:G:6511:ARG:NH1	1:G:6513:TYR:O	2.52	0.41
1:H:7116:VAL:CG1	1:H:7117:GLY:N	2.82	0.41
1:H:7158:VAL:CG2	1:H:7199:LEU:HD23	2.48	0.41
1:H:7264:ARG:HG3	1:H:7265:PHE:N	2.35	0.41
1:H:7374:PRO:HG3	1:H:7380:ALA:CA	2.49	0.41
1:H:7523:SER:O	1:H:7524:ILE:C	2.59	0.41
1:A:133:LEU:HB2	1:A:199:LEU:HD11	2.02	0.41
1:B:1227:ARG:CG	1:B:1227:ARG:NH1	2.71	0.41
1:B:1360:SER:HA	1:B:1363:GLU:CD	2.41	0.41
1:B:1377:PHE:O	1:B:1378:GLU:C	2.57	0.41
1:C:2287:ALA:O	1:C:2288:LEU:C	2.58	0.41
1:C:2381:VAL:HG13	1:C:2407:MSE:CE	2.50	0.41
1:E:4061:GLN:HA	1:E:4064:GLN:HG3	2.02	0.41
1:E:4179:ILE:O	1:E:4182:GLY:N	2.53	0.41
1:E:4302:ILE:HA	1:E:4305:HIS:CE1	2.55	0.41
1:F:5177:MSE:HG3	1:F:5177:MSE:O	2.20	0.41
1:F:5439:GLY:HA3	1:F:5460:PHE:HE2	1.85	0.41
1:G:6082:TYR:O	1:G:6086:MSE:HB2	2.20	0.41
1:G:6434:TYR:O	1:G:6439:GLY:N	2.53	0.41
1:H:7060:THR:H	1:H:7063:ILE:HD12	1.84	0.41
1:H:7244:ASP:N	1:H:7248:ARG:HH12	2.14	0.41
1:H:7276:PHE:HD1	1:H:7281:GLN:OE1	2.03	0.41
1:H:7323:ILE:C	1:H:7325:MSE:N	2.71	0.41
1:H:7040:PHE:HE2	1:H:7565:LEU:CD1	2.33	0.41
1:A:112:TYR:OH	1:A:183:LYS:HE3	2.20	0.41
1:A:333:SER:O	1:A:334:GLU:C	2.57	0.41
1:A:421:ASN:HA	1:A:422:PRO:O	2.21	0.41
1:A:97:TYR:CE2	1:A:188:THR:HB	2.54	0.41
1:B:1333:SER:O	1:B:1334:GLU:C	2.59	0.41
1:B:1401:PRO:HA	1:B:1436:LEU:HD23	2.01	0.41
1:B:1431:GLU:O	1:B:1433:ALA:N	2.53	0.41
1:C:2085:ILE:C	1:C:2087:GLY:N	2.71	0.41
1:C:2176:GLY:C	1:C:2178:GLY:H	2.24	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2205:VAL:HG11	1:C:2231:TYR:CD1	2.55	0.41
1:C:2259:ASN:N	1:C:2259:ASN:ND2	2.68	0.41
1:C:2417:PHE:CE2	1:C:2444:ALA:CB	3.04	0.41
1:C:2507:LEU:HD13	1:C:2507:LEU:HA	1.88	0.41
1:D:3113:THR:HA	1:D:3114:PRO:HA	1.84	0.41
1:D:3120:CYS:O	1:D:3123:TYR:HB2	2.21	0.41
1:D:3184:LEU:HA	1:D:3184:LEU:HD12	1.90	0.41
1:E:4100:LEU:HD23	1:E:4189:ALA:HB2	2.01	0.41
1:E:4218:TYR:O	1:F:5057:LYS:HE2	2.20	0.41
1:E:4392:VAL:HG13	3:E:4601:NAD:O4D	2.20	0.41
1:F:5172:LEU:HD23	1:F:5172:LEU:HA	1.79	0.41
1:F:5336:GLU:HG3	1:F:5336:GLU:H	1.51	0.41
1:G:6028:LEU:HD21	1:G:6048:LEU:HD12	2.01	0.41
1:G:6150:TRP:CE2	1:G:6199:LEU:HD13	2.55	0.41
1:G:6182:GLY:O	1:G:6185:CYS:N	2.52	0.41
1:G:6374:PRO:CG	1:G:6380:ALA:HB2	2.49	0.41
1:G:6422:PRO:HB2	1:G:6423:THR:H	1.63	0.41
1:G:6396:GLY:HA2	1:G:6425:GLN:C	2.39	0.41
1:H:7108:MSE:HE2	1:H:7108:MSE:HB2	1.77	0.41
1:H:7159:VAL:CG2	1:H:7184:LEU:HD11	2.48	0.41
1:H:7238:PHE:CE1	1:H:7242:ILE:HG13	2.56	0.41
1:H:7548:ASP:OD1	1:H:7550:ALA:HB3	2.20	0.41
1:A:437:THR:HG21	1:A:441:CYS:HB3	2.03	0.41
1:A:519:ILE:HG13	1:A:519:ILE:O	2.20	0.41
1:A:545:GLU:HG3	1:A:549:LYS:HZ1	1.85	0.41
1:A:552:TYR:CE1	1:A:556:ARG:NE	2.89	0.41
1:B:1133:LEU:HB3	1:B:1201:VAL:HG13	2.02	0.41
1:C:2338:GLN:O	1:C:2367:HIS:CE1	2.74	0.41
1:D:3243:THR:CB	1:D:3248:ARG:HD2	2.37	0.41
1:D:3271:GLU:O	1:D:3485:HIS:NE2	2.53	0.41
1:D:3505:GLU:H	1:D:3505:GLU:CD	2.16	0.41
1:D:3506:GLU:HB3	1:D:3511:ARG:CD	2.51	0.41
1:D:3546:PRO:HG3	1:D:3552:TYR:CD1	2.56	0.41
1:E:4041:THR:HG23	1:E:4044:GLU:CD	2.41	0.41
1:E:4089:GLN:O	1:E:4091:ARG:N	2.51	0.41
1:E:4376:THR:O	1:E:4377:PHE:C	2.58	0.41
1:E:4454:LEU:HD11	1:E:4460:PHE:CE2	2.55	0.41
1:E:4535:TYR:HA	1:E:4535:TYR:HD2	1.73	0.41
1:F:5159:VAL:HG23	1:F:5184:LEU:HD11	2.01	0.41
1:F:5240:LYS:O	1:F:5241:ALA:C	2.58	0.41
1:G:6253:GLN:HG3	1:G:6276:PHE:CE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:6306:LYS:NZ	1:G:6384:LEU:O	2.52	0.41
1:H:7112:TYR:CG	1:H:7113:THR:N	2.85	0.41
1:H:7327:MSE:HE1	1:H:7337:ALA:C	2.40	0.41
1:H:7328:VAL:CG2	1:H:7334:GLU:N	2.83	0.41
1:H:7510:GLY:O	1:H:7512:LEU:CD1	2.68	0.41
1:A:108:MSE:HE2	1:A:108:MSE:HB2	1.84	0.41
1:A:166:ILE:HD13	1:A:256:ASP:CB	2.51	0.41
1:B:1069:HIS:C	1:B:1071:ASN:N	2.74	0.41
1:B:1218:TYR:HB3	1:B:1222:TYR:CE2	2.55	0.41
1:B:1265:PHE:HB3	1:B:1269:TYR:HE1	1.86	0.41
1:B:1363:GLU:C	1:B:1365:PHE:H	2.24	0.41
1:C:2171:ASP:O	1:C:2172:LEU:HD23	2.20	0.41
1:C:2470:ILE:O	1:C:2472:PRO:N	2.53	0.41
1:C:2552:TYR:CD1	1:C:2556:ARG:NH1	2.89	0.41
1:D:3377:PHE:O	1:D:3381:VAL:HG23	2.21	0.41
1:E:4209:ASN:O	1:E:4213:LEU:HD12	2.21	0.41
1:E:4165:ARG:CD	1:E:4259:ASN:HD21	2.33	0.41
1:E:4444:ALA:HB2	1:E:4512:LEU:HD13	2.02	0.41
1:E:4047:MSE:SE	1:E:4566:LEU:HD22	2.71	0.41
1:F:5041:THR:OG1	1:F:5042:LEU:N	2.54	0.41
1:G:6176:GLY:O	1:G:6177:MSE:C	2.58	0.41
1:H:7044:GLU:O	1:H:7048:LEU:HD23	2.20	0.41
1:H:7037:GLY:O	1:H:7054:LEU:HD13	2.20	0.41
1:H:7292:LEU:O	1:H:7295:GLN:N	2.54	0.41
1:H:7298:ILE:HA	1:H:7298:ILE:HD12	1.84	0.41
1:H:7402:ASP:C	1:H:7405:ARG:HG2	2.40	0.41
1:A:128:ARG:HG3	1:B:1091:ARG:CZ	2.50	0.41
1:A:238:PHE:CD2	1:A:238:PHE:C	2.94	0.41
1:A:373:ILE:HD12	1:A:373:ILE:N	2.34	0.41
1:A:535:TYR:O	1:A:538:LYS:HD3	2.20	0.41
1:B:1310:LEU:HD21	1:B:1398:LEU:CB	2.45	0.41
1:B:1491:PHE:O	1:B:1494:ALA:N	2.51	0.41
1:C:2313:GLY:O	1:C:2314:GLU:C	2.58	0.41
1:C:2380:ALA:O	1:C:2382:ASN:N	2.53	0.41
1:D:3176:GLY:O	1:D:3177:MSE:C	2.58	0.41
1:D:3304:GLU:O	1:D:3305:HIS:C	2.58	0.41
1:D:3529:LYS:HA	1:D:3532:GLU:CD	2.40	0.41
1:D:3094:LYS:NZ	1:D:3559:ARG:O	2.50	0.41
1:E:4055:PRO:O	1:E:4057:LYS:N	2.54	0.41
1:E:4107:LEU:HD13	1:E:4107:LEU:HA	1.78	0.41
1:F:5028:LEU:HD13	1:F:5028:LEU:HA	1.98	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:5278:ASP:O	1:F:5280:ILE:N	2.53	0.41
1:F:5416:ILE:O	1:F:5416:ILE:HG12	2.21	0.41
1:F:5531:THR:O	1:F:5534:LEU:HB2	2.20	0.41
1:G:6210:ILE:O	1:G:6214:LYS:HG3	2.21	0.41
1:G:6332:LEU:HD23	1:G:6337:ALA:N	2.36	0.41
1:G:6346:LYS:HB3	3:G:6601:NAD:C5A	2.50	0.41
1:H:7090:GLU:HG2	1:H:7131:LYS:HZ3	1.85	0.41
1:H:7179:ILE:CB	1:H:7180:PRO:CD	2.97	0.41
1:A:292:LEU:O	1:A:296:LYS:HB2	2.21	0.41
1:A:381:VAL:HG13	1:A:407:MSE:HE1	2.02	0.41
1:A:99:ILE:C	1:A:102:ASP:HB2	2.41	0.41
1:A:98:ARG:HG3	1:A:99:ILE:N	2.32	0.41
1:A:220:GLY:HA2	1:B:1056:PRO:HG2	2.03	0.41
1:B:1075:MSE:HG3	1:B:1080:GLU:HG2	2.02	0.41
1:B:1229:GLN:NE2	1:B:1229:GLN:HA	2.35	0.41
1:B:1322:LEU:O	1:B:1325:MSE:HB2	2.20	0.41
1:C:2069:HIS:O	1:C:2071:ASN:N	2.54	0.41
1:C:2310:LEU:C	1:C:2344:PHE:O	2.58	0.41
1:D:3116:VAL:HG13	1:D:3117:GLY:H	1.84	0.41
1:D:3137:ILE:C	1:D:3139:ASP:N	2.72	0.41
1:D:3298:ILE:HD12	1:D:3413:ARG:HD3	2.03	0.41
1:D:3307:ILE:CG2	1:D:3308:LEU:N	2.83	0.41
1:E:4135:ILE:CD1	1:E:4238:PHE:HD1	2.34	0.41
1:E:4175:TYR:CE2	1:E:4218:TYR:HD2	2.39	0.41
1:E:4336:GLU:HG3	1:E:4336:GLU:H	1.37	0.41
1:E:4303:SER:O	1:E:4340:LYS:HE2	2.20	0.41
1:E:4357:LYS:HD3	1:E:4357:LYS:HA	1.78	0.41
1:E:4422:PRO:HB2	1:E:4423:THR:H	1.60	0.41
1:E:4481:CYS:SG	1:E:4531:THR:HB	2.60	0.41
1:F:5024:LYS:HA	1:F:5028:LEU:CD2	2.51	0.41
1:G:6123:TYR:O	1:G:6125:HIS:N	2.54	0.41
1:G:6164:GLU:O	1:G:6171:ASP:N	2.54	0.41
1:G:6384:LEU:HA	1:G:6384:LEU:HD12	1.90	0.41
1:G:6382:ASN:O	1:G:6385:LYS:HE2	2.20	0.41
1:G:6471:PHE:CG	1:G:6472:PRO:CD	3.00	0.41
1:H:7144:ARG:HA	1:H:7144:ARG:HD2	1.86	0.41
1:H:7266:LEU:HD12	1:H:7266:LEU:C	2.40	0.41
1:H:7319:ILE:O	1:H:7321:ASN:N	2.54	0.41
1:A:183:LYS:HD3	1:A:183:LYS:HA	1.63	0.41
1:A:243:THR:CB	1:A:248:ARG:HD2	2.12	0.41
1:A:363:GLU:HB2	1:A:364:PRO:HD3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:384:LEU:O	1:A:385:LYS:HB2	2.21	0.41
1:A:298:ILE:CD1	1:A:413:ARG:HD3	2.51	0.41
1:A:478:VAL:HG13	1:A:483:THR:HB	2.02	0.41
1:A:536:ALA:O	1:A:538:LYS:HE2	2.20	0.41
1:A:541:PHE:N	1:A:541:PHE:HD2	2.19	0.41
1:B:1066:LEU:HD11	1:B:1070:ARG:HH11	1.86	0.41
1:B:1400:THR:O	1:B:1404:ILE:HG13	2.20	0.41
1:B:1469:TYR:CZ	1:B:1516:LEU:HD13	2.56	0.41
1:C:2174:VAL:HG23	1:C:2174:VAL:O	2.21	0.41
1:C:2388:THR:CG2	1:C:2415:VAL:HB	2.41	0.41
1:C:2054:LEU:HD23	1:D:3130:PRO:HG2	2.03	0.41
1:D:3154:HIS:O	1:D:3197:ARG:CD	2.69	0.41
1:D:3307:ILE:HG22	1:D:3308:LEU:N	2.36	0.41
1:D:3308:LEU:CD1	1:D:3342:TRP:HB2	2.47	0.41
1:E:4212:LEU:O	1:E:4215:ASP:N	2.35	0.41
1:E:4291:LEU:O	1:E:4294:ALA:HB3	2.21	0.41
1:E:4429:THR:HB	1:E:4449:PHE:HE2	1.85	0.41
1:F:5212:LEU:C	1:F:5214:LYS:N	2.73	0.41
1:F:5206:GLY:CA	1:F:5223:GLN:HE21	2.34	0.41
1:F:5255:GLU:O	1:F:5257:PHE:CD1	2.74	0.41
1:F:5260:HIS:C	1:F:5260:HIS:ND1	2.74	0.41
1:G:6217:PHE:CZ	1:H:7067:ARG:HA	2.56	0.41
1:G:6252:ILE:O	1:G:6275:THR:OG1	2.37	0.41
1:G:6421:ASN:C	1:G:6425:GLN:HB2	2.41	0.41
1:H:7031:ASN:HA	1:H:7032:PRO:HD2	1.85	0.41
1:H:7261:ASN:HA	1:H:7264:ARG:HG2	2.03	0.41
1:A:363:GLU:O	1:A:364:PRO:C	2.59	0.41
1:A:325:MSE:HB3	1:A:492:LEU:HD13	2.02	0.41
1:A:492:LEU:O	1:A:495:ALA:HB3	2.21	0.41
1:A:535:TYR:CZ	1:A:545:GLU:HA	2.56	0.41
1:B:1140:ARG:NH1	1:B:1230:GLN:HG2	2.36	0.41
1:B:1298:ILE:HA	1:B:1298:ILE:HD12	1.90	0.41
1:B:1300:LYS:C	1:B:1304:GLU:OE1	2.60	0.41
1:B:1310:LEU:CD2	1:B:1399:PHE:CE2	3.03	0.41
1:B:1409:SER:OG	1:B:1410:ILE:N	2.54	0.41
1:B:1420:SER:OG	1:B:1427:GLU:OE1	2.39	0.41
1:C:2160:VAL:HG12	1:C:2201:VAL:CB	2.47	0.41
1:C:2161:THR:HA	1:C:2257:PHE:CE1	2.55	0.41
1:C:2232:ASP:OD2	1:C:2232:ASP:N	2.37	0.41
1:C:2468:VAL:HA	1:C:2471:PHE:CE2	2.56	0.41
1:D:3166:ILE:O	1:D:3167:LEU:C	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3183:LYS:HD2	1:D:3255:GLU:OE2	2.20	0.41
1:D:3302:ILE:CD1	1:D:3330:ASN:HD22	2.33	0.41
1:E:4026:LYS:C	1:E:4028:LEU:H	2.23	0.41
1:E:4116:VAL:CG2	1:E:4179:ILE:HD13	2.42	0.41
1:E:4239:MSE:HB3	1:E:4273:TYR:CE1	2.56	0.41
1:F:5319:ILE:O	1:F:5320:ALA:C	2.58	0.41
1:G:6140:ARG:O	1:G:6140:ARG:HG3	2.21	0.41
1:G:6243:THR:HG22	1:G:6247:GLY:O	2.20	0.41
1:G:6313:GLY:HA3	3:G:6601:NAD:O5B	2.20	0.41
1:G:6332:LEU:CD2	1:G:6337:ALA:HA	2.51	0.41
1:G:6374:PRO:HG3	1:G:6380:ALA:CB	2.51	0.41
1:G:6416:ILE:HG12	1:G:6416:ILE:O	2.20	0.41
1:G:6470:ILE:O	1:G:6471:PHE:C	2.59	0.41
1:H:7113:THR:HA	1:H:7116:VAL:HG12	2.03	0.41
1:H:7176:GLY:C	1:H:7178:GLY:N	2.74	0.41
1:H:7174:VAL:HG21	1:H:7219:MSE:HB2	2.03	0.41
1:H:7276:PHE:CG	1:H:7276:PHE:O	2.74	0.41
1:H:7470:ILE:HG22	1:H:7471:PHE:N	2.35	0.41
1:H:7552:TYR:CE1	1:H:7556:ARG:HD2	2.56	0.41
1:A:105:GLU:HA	1:A:108:MSE:CE	2.51	0.41
1:A:159:VAL:HG21	1:A:184:LEU:HD13	2.03	0.41
1:A:503:THR:O	1:A:506:GLU:N	2.54	0.41
1:B:1140:ARG:HB2	1:B:1140:ARG:HE	1.42	0.41
1:B:1144:ARG:HH11	1:B:1244:ASP:CB	2.32	0.41
1:B:1215:ASP:HB3	1:B:1218:TYR:HB2	2.03	0.41
1:B:1253:GLN:NE2	1:B:1254:PHE:O	2.54	0.41
1:B:1490:VAL:O	1:B:1494:ALA:N	2.54	0.41
1:C:2038:MSE:HB3	1:C:2059:GLU:HG3	2.00	0.41
1:C:2079:LEU:O	1:C:2082:TYR:HB3	2.21	0.41
1:C:2301:PRO:O	1:C:2304:GLU:OE2	2.39	0.41
1:C:2308:LEU:HD12	1:C:2342:TRP:O	2.21	0.41
1:C:2404:ILE:HD13	1:C:2433:ALA:HA	2.02	0.41
1:C:2431:GLU:O	1:C:2432:GLU:C	2.57	0.41
1:C:2470:ILE:C	1:C:2472:PRO:HD2	2.41	0.41
1:D:3079:LEU:HD11	1:D:3119:ALA:CA	2.49	0.41
1:D:3133:LEU:HD13	1:D:3133:LEU:HA	1.78	0.41
1:E:4165:ARG:HB2	1:E:4257:PHE:O	2.21	0.41
1:E:4166:ILE:HD13	1:E:4166:ILE:HA	1.74	0.41
1:E:4380:ALA:O	1:E:4381:VAL:C	2.59	0.41
1:E:4396:GLY:HA2	1:E:4425:GLN:CA	2.48	0.41
1:G:6061:GLN:HA	1:G:6064:GLN:NE2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:6128:ARG:HG3	1:H:7091:ARG:NH1	2.36	0.41
1:G:6235:ILE:HG12	1:G:6235:ILE:H	1.64	0.41
1:G:6474:VAL:O	1:G:6477:ALA:N	2.54	0.41
1:G:6543:TYR:HA	1:G:6544:PRO:C	2.41	0.41
1:H:7099:ILE:O	1:H:7100:LEU:C	2.60	0.41
1:H:7255:GLU:O	1:H:7257:PHE:CD1	2.74	0.41
1:A:267:ARG:NH1	1:A:267:ARG:CG	2.84	0.40
1:A:28:LEU:HA	1:A:28:LEU:HD12	1.88	0.40
1:A:291:LEU:HD12	1:A:323:ILE:HD11	2.03	0.40
1:A:389:ILE:O	1:A:389:ILE:CG2	2.69	0.40
1:B:1210:ILE:CA	1:B:1213:LEU:HD12	2.34	0.40
1:B:1252:ILE:O	1:B:1275:THR:HA	2.21	0.40
1:B:1376:THR:HB	1:B:1379:ASP:CB	2.50	0.40
1:B:1429:THR:HG23	1:B:1432:GLU:CD	2.42	0.40
1:C:2036:LYS:O	1:C:2039:ALA:HB3	2.22	0.40
1:C:2044:GLU:C	1:C:2048:LEU:HD23	2.41	0.40
1:C:2097:TYR:HA	1:C:2100:LEU:HB2	2.02	0.40
1:C:2289:ALA:O	1:C:2499:THR:OG1	2.37	0.40
1:C:2402:ASP:CA	1:C:2405:ARG:HG2	2.49	0.40
1:C:2408:ALA:HA	1:C:2414:PRO:HG3	2.03	0.40
1:C:2429:THR:HA	1:C:2449:PHE:CE1	2.56	0.40
1:D:3143:VAL:O	1:D:3144:ARG:C	2.60	0.40
1:D:3146:ILE:O	1:D:3147:VAL:C	2.60	0.40
1:D:3183:LYS:CE	1:D:3255:GLU:OE2	2.70	0.40
1:E:4059:GLU:CG	1:E:4063:ILE:HG21	2.46	0.40
1:E:4266:LEU:HD12	1:E:4270:ARG:HB2	2.03	0.40
1:E:4308:LEU:HD12	1:E:4309:PHE:N	2.34	0.40
1:E:4346:LYS:O	1:E:4346:LYS:HG2	2.19	0.40
1:F:5503:THR:O	1:F:5507:LEU:HD22	2.21	0.40
1:G:6300:LYS:HD2	1:G:6304:GLU:CB	2.49	0.40
1:G:6359:ASP:OD2	1:G:6359:ASP:O	2.40	0.40
1:G:6374:PRO:CB	1:G:6383:ILE:HD12	2.50	0.40
1:G:6306:LYS:CE	1:G:6384:LEU:O	2.69	0.40
1:G:6478:VAL:CG1	1:G:6479:ILE:N	2.82	0.40
1:G:6487:SER:OG	1:G:6539:MSE:HE1	2.20	0.40
1:H:7269:TYR:HB3	1:H:7273:TYR:CD1	2.48	0.40
1:H:7454:LEU:H	1:H:7454:LEU:HD12	1.86	0.40
1:H:7454:LEU:HD12	1:H:7458:ARG:HB2	2.03	0.40
1:A:354:ARG:NE	1:A:356:ALA:HB3	2.37	0.40
1:A:401:PRO:HB3	1:A:436:LEU:CD2	2.47	0.40
1:A:468:VAL:HA	1:A:471:PHE:CE2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:470:ILE:HG22	1:A:471:PHE:N	2.36	0.40
1:B:1066:LEU:O	1:B:1066:LEU:HD12	2.21	0.40
1:B:1147:VAL:O	1:B:1149:ASN:N	2.54	0.40
1:B:1396:GLY:HA2	1:B:1425:GLN:HA	2.04	0.40
1:C:2210:ILE:O	1:C:2214:LYS:HD2	2.21	0.40
1:D:3065:ALA:O	1:D:3066:LEU:C	2.60	0.40
1:D:3333:SER:HB3	1:D:3336:GLU:CG	2.51	0.40
1:D:3376:THR:CG2	1:D:3377:PHE:N	2.84	0.40
1:E:4242:ILE:HG22	1:E:4243:THR:N	2.36	0.40
1:E:4401:PRO:HA	1:E:4404:ILE:HD12	2.03	0.40
1:F:5284:ALA:CB	1:F:5319:ILE:HA	2.50	0.40
1:F:5520:GLN:O	1:F:5523:SER:N	2.55	0.40
1:G:6079:LEU:HD13	1:G:6118:LEU:HB3	2.03	0.40
1:G:6240:LYS:O	1:G:6242:ILE:N	2.54	0.40
1:G:6319:ILE:HG22	1:G:6323:ILE:HD11	2.03	0.40
1:G:6447:SER:HB3	1:G:6448:PRO:HD2	2.02	0.40
1:H:7466:ASN:C	1:H:7468:VAL:H	2.25	0.40
1:A:155:VAL:HA	1:A:197:ARG:O	2.21	0.40
1:A:95:LEU:HG	1:A:99:ILE:HD12	2.03	0.40
1:B:1292:LEU:HD23	1:B:1292:LEU:HA	1.81	0.40
1:C:2072:LEU:HA	1:C:2072:LEU:HD12	1.82	0.40
1:C:2119:ALA:O	1:C:2123:TYR:N	2.54	0.40
1:C:2289:ALA:O	1:C:2292:LEU:HB2	2.21	0.40
1:D:3100:LEU:C	1:D:3102:ASP:N	2.73	0.40
1:D:3169:LEU:CD2	1:D:3172:LEU:HD11	2.50	0.40
1:D:3137:ILE:HG22	1:D:3221:LEU:HD23	2.02	0.40
1:D:3394:GLY:O	1:D:3425:GLN:CG	2.65	0.40
1:D:3400:THR:OG1	1:D:3402:ASP:HB2	2.21	0.40
1:D:3477:ALA:HB1	1:D:3531:THR:CG2	2.44	0.40
1:E:4136:SER:HB2	1:E:4221:LEU:HD21	2.02	0.40
1:E:4166:ILE:O	1:E:4167:LEU:O	2.40	0.40
1:E:4356:ALA:HA	1:E:4357:LYS:HZ2	1.86	0.40
1:E:4404:ILE:O	1:E:4405:ARG:C	2.59	0.40
1:F:5026:LYS:O	1:F:5027:PRO:C	2.57	0.40
1:E:4056:PRO:HD3	1:F:5134:PHE:HB3	2.03	0.40
1:F:5240:LYS:HG2	1:F:5244:ASP:OD1	2.21	0.40
1:F:5360:SER:OG	1:F:5361:TYR:N	2.54	0.40
1:F:5412:GLU:HA	1:F:5440:ARG:NH1	2.36	0.40
1:G:6165:ARG:CZ	1:G:6259:ASN:ND2	2.85	0.40
1:G:6419:LEU:O	1:G:6446:GLY:HA3	2.21	0.40
1:H:7104:ILE:HG23	1:H:7105:GLU:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:7262:ALA:HB1	1:H:7277:ASN:ND2	2.36	0.40
1:H:7468:VAL:O	1:H:7468:VAL:CG2	2.67	0.40
1:A:532:GLU:HG2	1:A:549:LYS:HG2	2.03	0.40
1:B:1243:THR:O	1:B:1247:GLY:O	2.39	0.40
1:B:1300:LYS:NZ	1:B:1387:SER:CB	2.84	0.40
1:C:2321:ASN:C	1:C:2323:ILE:N	2.73	0.40
1:C:2546:PRO:O	1:C:2549:LYS:HE3	2.20	0.40
1:D:3072:LEU:HA	1:D:3075:MSE:CE	2.44	0.40
1:C:2129:ARG:NH2	1:D:3091:ARG:HG3	2.35	0.40
1:D:3243:THR:CB	1:D:3248:ARG:HH11	2.35	0.40
1:D:3266:LEU:O	1:D:3270:ARG:CB	2.70	0.40
1:D:3370:PRO:O	1:D:3372:SER:N	2.55	0.40
1:D:3404:ILE:HG21	1:D:3436:LEU:CB	2.52	0.40
1:D:3420:SER:HB3	1:D:3425:GLN:O	2.22	0.40
1:D:3511:ARG:H	1:D:3511:ARG:HG3	1.53	0.40
1:E:4068:PHE:CE2	1:E:4072:LEU:HD22	2.56	0.40
1:E:4174:VAL:HG21	1:E:4219:MSE:HB2	2.03	0.40
1:E:4435:THR:C	1:E:4437:THR:H	2.23	0.40
1:E:4281:GLN:HB3	1:E:4491:PHE:CE1	2.57	0.40
1:E:4477:ALA:HB2	1:E:4527:ALA:O	2.22	0.40
1:F:5107:LEU:HD13	1:F:5107:LEU:HA	1.85	0.40
1:F:5266:LEU:HD12	1:F:5266:LEU:C	2.42	0.40
1:F:5317:LEU:H	1:F:5317:LEU:CD1	2.05	0.40
1:F:5419:LEU:CA	1:F:5446:GLY:HA3	2.49	0.40
1:F:5522:VAL:O	1:F:5526:ILE:HG13	2.21	0.40
1:F:5568:ASP:OD1	1:F:5570:TYR:HD2	2.05	0.40
1:G:6205:VAL:HG11	1:G:6231:TYR:CD1	2.53	0.40
1:G:6308:LEU:HB3	1:G:6389:ILE:CD1	2.51	0.40
1:H:7377:PHE:O	1:H:7380:ALA:N	2.54	0.40
1:H:7400:THR:OG1	1:H:7402:ASP:HB2	2.20	0.40
1:H:7511:ARG:HB3	1:H:7511:ARG:NH1	2.37	0.40
1:A:323:ILE:HG22	1:A:324:VAL:N	2.37	0.40
1:A:432:GLU:H	1:A:432:GLU:HG2	1.76	0.40
1:A:453:LYS:HD3	1:A:454:LEU:O	2.21	0.40
1:A:81:LYS:O	1:A:82:TYR:C	2.60	0.40
1:B:1030:LEU:HD23	1:B:1030:LEU:HA	1.87	0.40
1:B:1339:LYS:CA	1:B:1367:HIS:NE2	2.81	0.40
1:B:1453:LYS:HA	1:B:1459:VAL:HA	2.03	0.40
1:C:2298:ILE:HG22	1:C:2300:LYS:N	2.37	0.40
1:C:2480:LEU:HD21	1:C:2556:ARG:CB	2.52	0.40
1:D:3112:TYR:CG	1:D:3113:THR:N	2.89	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3199:LEU:HD12	1:D:3199:LEU:C	2.42	0.40
1:D:3288:LEU:HG	1:D:3292:LEU:CD2	2.51	0.40
1:D:3506:GLU:HA	1:D:3511:ARG:HD2	2.03	0.40
1:E:4137:ILE:HB	1:E:4205:VAL:HG12	2.04	0.40
1:E:4336:GLU:HA	1:E:4339:LYS:HB2	2.03	0.40
1:E:4439:GLY:HA3	1:E:4460:PHE:HE2	1.86	0.40
1:E:4512:LEU:O	1:E:4513:TYR:CD2	2.74	0.40
1:E:4530:VAL:O	1:E:4531:THR:C	2.60	0.40
1:G:6140:ARG:HB2	1:G:6140:ARG:HE	1.62	0.40
1:G:6259:ASN:O	1:G:6260:HIS:C	2.59	0.40
1:G:6430:ALA:O	1:G:6431:GLU:C	2.60	0.40
1:H:7107:LEU:O	1:H:7108:MSE:C	2.60	0.40
1:H:7159:VAL:CG2	1:H:7184:LEU:CD1	2.99	0.40
1:H:7210:ILE:O	1:H:7213:LEU:N	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	549/584 (94%)	415 (76%)	99 (18%)	35 (6%)	1	4
1	B	549/584 (94%)	406 (74%)	107 (20%)	36 (7%)	1	3
1	C	549/584 (94%)	407 (74%)	102 (19%)	40 (7%)	1	3
1	D	549/584 (94%)	394 (72%)	119 (22%)	36 (7%)	1	3
1	E	549/584 (94%)	429 (78%)	94 (17%)	26 (5%)	2	8
1	F	549/584 (94%)	437 (80%)	83 (15%)	29 (5%)	2	6
1	G	549/584 (94%)	398 (72%)	111 (20%)	40 (7%)	1	3
1	H	549/584 (94%)	398 (72%)	120 (22%)	31 (6%)	2	5
All	All	4392/4672 (94%)	3284 (75%)	835 (19%)	273 (6%)	1	4

All (273) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	104	ILE
1	A	167	LEU
1	A	256	ASP
1	A	259	ASN
1	A	268	LYS
1	A	301	PRO
1	A	302	ILE
1	A	314	GLU
1	A	324	VAL
1	B	1093	GLU
1	B	1100	LEU
1	B	1127	PHE
1	B	1260	HIS
1	B	1268	LYS
1	B	1302	ILE
1	B	1303	SER
1	B	1451	PRO
1	B	1556	ARG
1	C	2259	ASN
1	C	2301	PRO
1	C	2302	ILE
1	C	2314	GLU
1	C	2423	THR
1	C	2455	THR
1	C	2520	GLN
1	C	2528	ILE
1	C	2570	TYR
1	D	3123	TYR
1	D	3229	GLN
1	D	3256	ASP
1	D	3259	ASN
1	D	3268	LYS
1	D	3284	ALA
1	D	3285	ALA
1	D	3301	PRO
1	D	3302	ILE
1	D	3303	SER
1	D	3314	GLU
1	D	3422	PRO
1	E	4167	LEU
1	E	4259	ASN
1	E	4302	ILE

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Mol	Chain	Res	Type
1	E	4422	PRO
1	F	5242	ILE
1	F	5256	ASP
1	F	5301	PRO
1	F	5302	ILE
1	F	5303	SER
1	F	5332	LEU
1	G	6256	ASP
1	G	6259	ASN
1	G	6301	PRO
1	G	6302	ILE
1	G	6303	SER
1	G	6393	ALA
1	G	6479	ILE
1	G	6562	TYR
1	H	7104	ILE
1	H	7256	ASP
1	H	7259	ASN
1	H	7301	PRO
1	H	7302	ILE
1	H	7303	SER
1	H	7314	GLU
1	H	7410	ILE
1	H	7423	THR
1	A	90	GLU
1	A	228	THR
1	A	244	ASP
1	A	320	ALA
1	A	347	TYR
1	A	371	GLU
1	A	383	ILE
1	A	479	ILE
1	A	500	SER
1	B	1094	LYS
1	B	1301	PRO
1	B	1314	GLU
1	B	1371	GLU
1	C	2293	ALA
1	C	2381	VAL
1	C	2382	ASN
1	C	2383	ILE
1	C	2500	SER

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Mol	Chain	Res	Type
1	C	2529	LYS
1	D	3096	PHE
1	D	3171	ASP
1	D	3305	HIS
1	D	3371	GLU
1	D	3420	SER
1	D	3433	ALA
1	D	3480	LEU
1	D	3554	LYS
1	E	4038	MSE
1	E	4090	GLU
1	E	4123	TYR
1	E	4213	LEU
1	E	4301	PRO
1	E	4305	HIS
1	E	4314	GLU
1	E	4334	GLU
1	E	4345	ASP
1	E	4354	ARG
1	E	4371	GLU
1	E	4404	ILE
1	E	4455	THR
1	F	5259	ASN
1	F	5283	THR
1	F	5314	GLU
1	F	5354	ARG
1	F	5432	GLU
1	F	5451	PRO
1	G	6231	TYR
1	G	6314	GLU
1	G	6363	GLU
1	G	6432	GLU
1	G	6509	GLN
1	H	7086	MSE
1	H	7090	GLU
1	H	7279	ASP
1	H	7409	SER
1	H	7554	LYS
1	A	397	ARG
1	A	432	GLU
1	B	1148	ASP
1	B	1222	TYR

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Mol	Chain	Res	Type
1	B	1228	THR
1	B	1259	ASN
1	B	1280	ILE
1	B	1284	ALA
1	B	1436	LEU
1	B	1554	LYS
1	C	2039	ALA
1	C	2225	ARG
1	C	2256	ASP
1	C	2260	HIS
1	C	2279	ASP
1	C	2292	LEU
1	C	2405	ARG
1	C	2426	ALA
1	C	2498	LEU
1	C	2527	ALA
1	C	2554	LYS
1	C	2562	TYR
1	D	3138	SER
1	D	3143	VAL
1	D	3230	GLN
1	D	3239	MSE
1	D	3552	TYR
1	E	4230	GLN
1	E	4520	GLN
1	E	4554	LYS
1	F	5093	GLU
1	F	5279	ASP
1	F	5423	THR
1	F	5498	LEU
1	F	5520	GLN
1	G	6067	ARG
1	G	6127	PHE
1	G	6213	LEU
1	G	6261	ASN
1	G	6284	ALA
1	G	6370	PRO
1	G	6488	ASP
1	G	6497	ALA
1	G	6520	GLN
1	H	7177	MSE
1	H	7228	THR

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Mol	Chain	Res	Type
1	H	7230	GLN
1	H	7350	LEU
1	H	7532	GLU
1	A	38	MSE
1	A	89	GLN
1	A	177	MSE
1	A	325	MSE
1	A	352	LYS
1	A	428	CYS
1	A	431	GLU
1	B	1070	ARG
1	B	1319	ILE
1	B	1364	PRO
1	B	1472	PRO
1	B	1550	ALA
1	C	2056	PRO
1	C	2284	ALA
1	C	2347	TYR
1	C	2404	ILE
1	D	3404	ILE
1	D	3432	GLU
1	D	3520	GLN
1	E	4332	LEU
1	E	4438	GLU
1	E	4516	LEU
1	F	5143	VAL
1	F	5228	THR
1	F	5280	ILE
1	F	5284	ALA
1	F	5316	ALA
1	F	5431	GLU
1	G	6061	GLN
1	G	6224	LYS
1	G	6241	ALA
1	G	6268	LYS
1	G	6285	ALA
1	G	6422	PRO
1	G	6431	GLU
1	G	6451	PRO
1	G	6468	VAL
1	G	6496	LYS
1	G	6550	ALA

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Mol	Chain	Res	Type
1	H	7432	GLU
1	H	7500	SER
1	A	269	TYR
1	B	1285	ALA
1	B	1299	SER
1	B	1335	GLN
1	B	1337	ALA
1	B	1428	CYS
1	B	1522	VAL
1	C	2076	THR
1	C	2303	SER
1	C	2334	GLU
1	C	2356	ALA
1	C	2552	TYR
1	D	3095	LEU
1	D	3166	ILE
1	E	4228	THR
1	F	5213	LEU
1	F	5243	THR
1	F	5268	LYS
1	F	5436	LEU
1	G	6167	LEU
1	G	6331	GLY
1	H	7231	TYR
1	H	7324	VAL
1	H	7381	VAL
1	A	56	PRO
1	A	279	ASP
1	A	470	ILE
1	A	528	ILE
1	B	1320	ALA
1	B	1479	ILE
1	C	2163	GLY
1	C	2451	PRO
1	C	2471	PHE
1	D	3074	LYS
1	D	3167	LEU
1	D	3205	VAL
1	D	3530	VAL
1	F	5138	SER
1	F	5404	ILE
1	G	6151	PRO

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Mol	Chain	Res	Type
1	G	6153	ASN
1	G	6471	PHE
1	H	7244	ASP
1	H	7280	ILE
1	A	323	ILE
1	E	4392	VAL
1	H	7478	VAL
1	A	451	PRO
1	D	3077	SER
1	H	7173	GLY
1	H	7553	VAL
1	G	6519	ILE
1	H	7522	VAL
1	B	1181	VAL
1	B	1404	ILE
1	D	3479	ILE
1	H	7143	VAL
1	A	143	VAL
1	C	2104	ILE
1	E	4381	VAL
1	G	6181	VAL

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	466/483 (96%)	332 (71%)	134 (29%)	0 1
1	B	466/483 (96%)	318 (68%)	148 (32%)	0 0
1	C	466/483 (96%)	327 (70%)	139 (30%)	0 1
1	D	466/483 (96%)	318 (68%)	148 (32%)	0 0
1	E	466/483 (96%)	340 (73%)	126 (27%)	0 1
1	F	466/483 (96%)	341 (73%)	125 (27%)	0 1
1	G	466/483 (96%)	335 (72%)	131 (28%)	0 1
1	H	466/483 (96%)	344 (74%)	122 (26%)	0 1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3728/3864 (96%)	2655 (71%)	1073 (29%)	0 1

All (1073) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	LYS
1	A	30	LEU
1	A	36	LYS
1	A	41	THR
1	A	51	GLN
1	A	56	PRO
1	A	57	LYS
1	A	62	ASP
1	A	63	ILE
1	A	66	LEU
1	A	70	ARG
1	A	71	ASN
1	A	74	LYS
1	A	75	MSE
1	A	77	SER
1	A	79	LEU
1	A	82	TYR
1	A	85	ILE
1	A	88	ILE
1	A	98	ARG
1	A	100	LEU
1	A	102	ASP
1	A	106	SER
1	A	107	LEU
1	A	108	MSE
1	A	113	THR
1	A	116	VAL
1	A	118	LEU
1	A	121	SER
1	A	123	TYR
1	A	128	ARG
1	A	136	SER
1	A	137	ILE
1	A	138	SER
1	A	152	GLU
1	A	154	HIS
1	A	156	LYS

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Mol	Chain	Res	Type
1	A	160	VAL
1	A	181	VAL
1	A	183	LYS
1	A	184	LEU
1	A	196	ASP
1	A	205	VAL
1	A	219	MSE
1	A	221	LEU
1	A	223	GLN
1	A	224	LYS
1	A	225	ARG
1	A	227	ARG
1	A	234	LEU
1	A	238	PHE
1	A	243	THR
1	A	245	ARG
1	A	259	ASN
1	A	261	ASN
1	A	263	PHE
1	A	267	ARG
1	A	270	ARG
1	A	286	VAL
1	A	298	ILE
1	A	299	SER
1	A	300	LYS
1	A	303	SER
1	A	304	GLU
1	A	317	LEU
1	A	323	ILE
1	A	332	LEU
1	A	333	SER
1	A	335	GLN
1	A	336	GLU
1	A	338	GLN
1	A	340	LYS
1	A	341	ILE
1	A	346	LYS
1	A	349	LEU
1	A	358	ILE
1	A	359	ASP
1	A	360	SER
1	A	363	GLU

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Mol	Chain	Res	Type
1	A	366	THR
1	A	368	SER
1	A	371	GLU
1	A	376	THR
1	A	378	GLU
1	A	383	ILE
1	A	384	LEU
1	A	385	LYS
1	A	387	SER
1	A	388	THR
1	A	389	ILE
1	A	397	ARG
1	A	400	THR
1	A	403	VAL
1	A	405	ARG
1	A	410	ILE
1	A	413	ARG
1	A	415	VAL
1	A	416	ILE
1	A	419	LEU
1	A	428	CYS
1	A	429	THR
1	A	431	GLU
1	A	440	ARG
1	A	447	SER
1	A	453	LYS
1	A	454	LEU
1	A	455	THR
1	A	456	ASP
1	A	458	ARG
1	A	464	GLN
1	A	476	LEU
1	A	480	LEU
1	A	483	THR
1	A	486	ILE
1	A	487	SER
1	A	488	ASP
1	A	496	LYS
1	A	502	LEU
1	A	504	ASP
1	A	507	LEU
1	A	511	ARG

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Mol	Chain	Res	Type
1	A	512	LEU
1	A	518	ASN
1	A	525	ASN
1	A	531	THR
1	A	535	TYR
1	A	539	MSE
1	A	547	GLU
1	A	551	LYS
1	A	559	ARG
1	A	561	GLU
1	A	565	LEU
1	A	571	GLU
1	A	572	TRP
1	B	1030	LEU
1	B	1033	ARG
1	B	1041	THR
1	B	1045	ARG
1	B	1057	LYS
1	B	1059	GLU
1	B	1070	ARG
1	B	1071	ASN
1	B	1073	LYS
1	B	1075	MSE
1	B	1076	THR
1	B	1077	SER
1	B	1085	ILE
1	B	1098	ARG
1	B	1100	LEU
1	B	1101	GLN
1	B	1102	ASP
1	B	1106	SER
1	B	1107	LEU
1	B	1108	MSE
1	B	1118	LEU
1	B	1121	SER
1	B	1123	TYR
1	B	1125	HIS
1	B	1131	LYS
1	B	1136	SER
1	B	1137	ILE
1	B	1138	SER
1	B	1140	ARG

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Mol	Chain	Res	Type
1	B	1146	ILE
1	B	1152	GLU
1	B	1154	HIS
1	B	1160	VAL
1	B	1171	ASP
1	B	1172	LEU
1	B	1183	LYS
1	B	1184	LEU
1	B	1194	ARG
1	B	1196	ASP
1	B	1205	VAL
1	B	1208	ASP
1	B	1214	LYS
1	B	1219	MSE
1	B	1221	LEU
1	B	1223	GLN
1	B	1226	ASP
1	B	1227	ARG
1	B	1228	THR
1	B	1232	ASP
1	B	1234	LEU
1	B	1237	GLU
1	B	1243	THR
1	B	1259	ASN
1	B	1261	ASN
1	B	1264	ARG
1	B	1266	LEU
1	B	1267	ARG
1	B	1270	ARG
1	B	1271	GLU
1	B	1272	LYS
1	B	1276	PHE
1	B	1278	ASP
1	B	1286	VAL
1	B	1297	VAL
1	B	1298	ILE
1	B	1299	SER
1	B	1303	SER
1	B	1304	GLU
1	B	1306	LYS
1	B	1317	LEU
1	B	1325	MSE

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Mol	Chain	Res	Type
1	B	1326	SER
1	B	1332	LEU
1	B	1333	SER
1	B	1336	GLU
1	B	1338	GLN
1	B	1339	LYS
1	B	1340	LYS
1	B	1343	MSE
1	B	1346	LYS
1	B	1349	LEU
1	B	1351	VAL
1	B	1355	LYS
1	B	1359	ASP
1	B	1360	SER
1	B	1363	GLU
1	B	1368	SER
1	B	1371	GLU
1	B	1373	ILE
1	B	1375	ASP
1	B	1384	LEU
1	B	1385	LYS
1	B	1388	THR
1	B	1397	ARG
1	B	1400	THR
1	B	1405	ARG
1	B	1409	SER
1	B	1411	ASN
1	B	1412	GLU
1	B	1413	ARG
1	B	1415	VAL
1	B	1416	ILE
1	B	1419	LEU
1	B	1423	THR
1	B	1425	GLN
1	B	1427	GLU
1	B	1429	THR
1	B	1440	ARG
1	B	1452	VAL
1	B	1453	LYS
1	B	1454	LEU
1	B	1455	THR
1	B	1456	ASP

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Mol	Chain	Res	Type
1	B	1458	ARG
1	B	1459	VAL
1	B	1467	ASN
1	B	1480	LEU
1	B	1482	ASN
1	B	1487	SER
1	B	1489	SER
1	B	1496	LYS
1	B	1500	SER
1	B	1501	GLN
1	B	1502	LEU
1	B	1504	ASP
1	B	1505	GLU
1	B	1506	GLU
1	B	1507	LEU
1	B	1509	GLN
1	B	1511	ARG
1	B	1512	LEU
1	B	1521	GLU
1	B	1523	SER
1	B	1525	ASN
1	B	1529	LYS
1	B	1531	THR
1	B	1532	GLU
1	B	1535	TYR
1	B	1537	ASN
1	B	1539	MSE
1	B	1543	TYR
1	B	1547	GLU
1	B	1549	LYS
1	B	1551	LYS
1	B	1555	GLU
1	B	1559	ARG
1	B	1561	GLU
1	B	1572	TRP
1	C	2024	LYS
1	C	2028	LEU
1	C	2030	LEU
1	C	2038	MSE
1	C	2041	THR
1	C	2048	LEU
1	C	2051	GLN

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Mol	Chain	Res	Type
1	C	2057	LYS
1	C	2070	ARG
1	C	2071	ASN
1	C	2075	MSE
1	C	2077	SER
1	C	2082	TYR
1	C	2086	MSE
1	C	2088	ILE
1	C	2093	GLU
1	C	2098	ARG
1	C	2100	LEU
1	C	2102	ASP
1	C	2104	ILE
1	C	2107	LEU
1	C	2118	LEU
1	C	2121	SER
1	C	2123	TYR
1	C	2128	ARG
1	C	2129	ARG
1	C	2136	SER
1	C	2138	SER
1	C	2140	ARG
1	C	2154	HIS
1	C	2156	LYS
1	C	2172	LEU
1	C	2175	TYR
1	C	2183	LYS
1	C	2184	LEU
1	C	2190	CYS
1	C	2194	ARG
1	C	2196	ASP
1	C	2197	ARG
1	C	2205	VAL
1	C	2212	LEU
1	C	2214	LYS
1	C	2221	LEU
1	C	2223	GLN
1	C	2224	LYS
1	C	2225	ARG
1	C	2227	ARG
1	C	2232	ASP
1	C	2234	LEU

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Mol	Chain	Res	Type
1	C	2235	ILE
1	C	2238	PHE
1	C	2243	THR
1	C	2250	THR
1	C	2253	GLN
1	C	2255	GLU
1	C	2259	ASN
1	C	2261	ASN
1	C	2267	ARG
1	C	2270	ARG
1	C	2275	THR
1	C	2286	VAL
1	C	2292	LEU
1	C	2298	ILE
1	C	2299	SER
1	C	2303	SER
1	C	2304	GLU
1	C	2306	LYS
1	C	2325	MSE
1	C	2329	GLU
1	C	2332	LEU
1	C	2333	SER
1	C	2338	GLN
1	C	2339	LYS
1	C	2341	ILE
1	C	2343	MSE
1	C	2349	LEU
1	C	2350	LEU
1	C	2351	VAL
1	C	2357	LYS
1	C	2358	ILE
1	C	2359	ASP
1	C	2363	GLU
1	C	2366	THR
1	C	2368	SER
1	C	2372	SER
1	C	2378	GLU
1	C	2379	ASP
1	C	2383	ILE
1	C	2384	LEU
1	C	2385	LYS
1	C	2388	THR

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Mol	Chain	Res	Type
1	C	2397	ARG
1	C	2400	THR
1	C	2405	ARG
1	C	2409	SER
1	C	2415	VAL
1	C	2416	ILE
1	C	2419	LEU
1	C	2425	GLN
1	C	2428	CYS
1	C	2429	THR
1	C	2431	GLU
1	C	2432	GLU
1	C	2447	SER
1	C	2449	PHE
1	C	2453	LYS
1	C	2454	LEU
1	C	2455	THR
1	C	2456	ASP
1	C	2458	ARG
1	C	2464	GLN
1	C	2481	CYS
1	C	2486	ILE
1	C	2492	LEU
1	C	2499	THR
1	C	2502	LEU
1	C	2504	ASP
1	C	2505	GLU
1	C	2506	GLU
1	C	2511	ARG
1	C	2516	LEU
1	C	2518	ASN
1	C	2519	ILE
1	C	2524	ILE
1	C	2529	LYS
1	C	2531	THR
1	C	2537	ASN
1	C	2538	LYS
1	C	2542	ARG
1	C	2543	TYR
1	C	2547	GLU
1	C	2549	LYS
1	C	2551	LYS

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Mol	Chain	Res	Type
1	C	2554	LYS
1	C	2556	ARG
1	C	2559	ARG
1	C	2561	GLU
1	C	2564	SER
1	C	2572	TRP
1	D	3023	GLU
1	D	3030	LEU
1	D	3033	ARG
1	D	3041	THR
1	D	3043	GLN
1	D	3057	LYS
1	D	3058	ILE
1	D	3070	ARG
1	D	3071	ASN
1	D	3072	LEU
1	D	3075	MSE
1	D	3077	SER
1	D	3085	ILE
1	D	3091	ARG
1	D	3098	ARG
1	D	3099	ILE
1	D	3101	GLN
1	D	3102	ASP
1	D	3106	SER
1	D	3107	LEU
1	D	3108	MSE
1	D	3118	LEU
1	D	3121	SER
1	D	3122	GLN
1	D	3123	TYR
1	D	3131	LYS
1	D	3133	LEU
1	D	3136	SER
1	D	3137	ILE
1	D	3140	ARG
1	D	3145	SER
1	D	3152	GLU
1	D	3156	LYS
1	D	3160	VAL
1	D	3162	ASP
1	D	3165	ARG

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Mol	Chain	Res	Type
1	D	3166	ILE
1	D	3181	VAL
1	D	3183	LYS
1	D	3184	LEU
1	D	3194	ARG
1	D	3196	ASP
1	D	3202	CYS
1	D	3204	ASP
1	D	3205	VAL
1	D	3210	ILE
1	D	3212	LEU
1	D	3214	LYS
1	D	3221	LEU
1	D	3223	GLN
1	D	3225	ARG
1	D	3228	THR
1	D	3232	ASP
1	D	3238	PHE
1	D	3243	THR
1	D	3244	ASP
1	D	3248	ARG
1	D	3252	ILE
1	D	3255	GLU
1	D	3257	PHE
1	D	3259	ASN
1	D	3261	ASN
1	D	3266	LEU
1	D	3267	ARG
1	D	3268	LYS
1	D	3270	ARG
1	D	3275	THR
1	D	3276	PHE
1	D	3278	ASP
1	D	3279	ASP
1	D	3286	VAL
1	D	3288	LEU
1	D	3292	LEU
1	D	3298	ILE
1	D	3299	SER
1	D	3300	LYS
1	D	3303	SER
1	D	3304	GLU

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Mol	Chain	Res	Type
1	D	3306	LYS
1	D	3332	LEU
1	D	3333	SER
1	D	3335	GLN
1	D	3336	GLU
1	D	3339	LYS
1	D	3346	LYS
1	D	3349	LEU
1	D	3351	VAL
1	D	3354	ARG
1	D	3355	LYS
1	D	3357	LYS
1	D	3359	ASP
1	D	3360	SER
1	D	3363	GLU
1	D	3367	HIS
1	D	3368	SER
1	D	3371	GLU
1	D	3372	SER
1	D	3375	ASP
1	D	3382	ASN
1	D	3383	ILE
1	D	3384	LEU
1	D	3385	LYS
1	D	3387	SER
1	D	3397	ARG
1	D	3400	THR
1	D	3405	ARG
1	D	3411	ASN
1	D	3413	ARG
1	D	3415	VAL
1	D	3416	ILE
1	D	3419	LEU
1	D	3425	GLN
1	D	3440	ARG
1	D	3447	SER
1	D	3453	LYS
1	D	3455	THR
1	D	3456	ASP
1	D	3458	ARG
1	D	3459	VAL
1	D	3481	CYS

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Mol	Chain	Res	Type
1	D	3482	ASN
1	D	3483	THR
1	D	3486	ILE
1	D	3487	SER
1	D	3492	LEU
1	D	3502	LEU
1	D	3504	ASP
1	D	3507	LEU
1	D	3511	ARG
1	D	3521	GLU
1	D	3525	ASN
1	D	3528	ILE
1	D	3529	LYS
1	D	3532	GLU
1	D	3535	TYR
1	D	3537	ASN
1	D	3538	LYS
1	D	3542	ARG
1	D	3543	TYR
1	D	3547	GLU
1	D	3549	LYS
1	D	3551	LYS
1	D	3556	ARG
1	D	3557	THR
1	D	3559	ARG
1	D	3561	GLU
1	D	3571	GLU
1	D	3572	TRP
1	E	4024	LYS
1	E	4028	LEU
1	E	4033	ARG
1	E	4041	THR
1	E	4043	GLN
1	E	4057	LYS
1	E	4058	ILE
1	E	4064	GLN
1	E	4070	ARG
1	E	4075	MSE
1	E	4076	THR
1	E	4098	ARG
1	E	4102	ASP
1	E	4108	MSE

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Mol	Chain	Res	Type
1	E	4118	LEU
1	E	4121	SER
1	E	4123	TYR
1	E	4125	HIS
1	E	4128	ARG
1	E	4129	ARG
1	E	4131	LYS
1	E	4136	SER
1	E	4138	SER
1	E	4145	SER
1	E	4152	GLU
1	E	4154	HIS
1	E	4156	LYS
1	E	4160	VAL
1	E	4166	ILE
1	E	4174	VAL
1	E	4181	VAL
1	E	4183	LYS
1	E	4184	LEU
1	E	4190	CYS
1	E	4194	ARG
1	E	4196	ASP
1	E	4199	LEU
1	E	4205	VAL
1	E	4214	LYS
1	E	4219	MSE
1	E	4221	LEU
1	E	4223	GLN
1	E	4225	ARG
1	E	4226	ASP
1	E	4227	ARG
1	E	4228	THR
1	E	4229	GLN
1	E	4236	ASP
1	E	4243	THR
1	E	4248	ARG
1	E	4250	THR
1	E	4253	GLN
1	E	4260	HIS
1	E	4261	ASN
1	E	4266	LEU
1	E	4267	ARG

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Mol	Chain	Res	Type
1	E	4270	ARG
1	E	4275	THR
1	E	4279	ASP
1	E	4286	VAL
1	E	4292	LEU
1	E	4296	LYS
1	E	4299	SER
1	E	4300	LYS
1	E	4303	SER
1	E	4304	GLU
1	E	4322	LEU
1	E	4326	SER
1	E	4328	VAL
1	E	4329	GLU
1	E	4336	GLU
1	E	4339	LYS
1	E	4345	ASP
1	E	4346	LYS
1	E	4350	LEU
1	E	4355	LYS
1	E	4357	LYS
1	E	4359	ASP
1	E	4360	SER
1	E	4363	GLU
1	E	4366	THR
1	E	4368	SER
1	E	4378	GLU
1	E	4384	LEU
1	E	4385	LYS
1	E	4387	SER
1	E	4397	ARG
1	E	4400	THR
1	E	4402	ASP
1	E	4405	ARG
1	E	4416	ILE
1	E	4419	LEU
1	E	4425	GLN
1	E	4428	CYS
1	E	4429	THR
1	E	4431	GLU
1	E	4438	GLU
1	E	4453	LYS

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Mol	Chain	Res	Type
1	E	4454	LEU
1	E	4458	ARG
1	E	4459	VAL
1	E	4486	ILE
1	E	4496	LYS
1	E	4499	THR
1	E	4501	GLN
1	E	4502	LEU
1	E	4503	THR
1	E	4506	GLU
1	E	4507	LEU
1	E	4511	ARG
1	E	4512	LEU
1	E	4518	ASN
1	E	4523	SER
1	E	4525	ASN
1	E	4528	ILE
1	E	4529	LYS
1	E	4534	LEU
1	E	4535	TYR
1	E	4537	ASN
1	E	4539	MSE
1	E	4549	LYS
1	E	4556	ARG
1	E	4559	ARG
1	E	4561	GLU
1	E	4571	GLU
1	E	4572	TRP
1	F	5028	LEU
1	F	5030	LEU
1	F	5033	ARG
1	F	5041	THR
1	F	5043	GLN
1	F	5045	ARG
1	F	5047	MSE
1	F	5048	LEU
1	F	5051	GLN
1	F	5057	LYS
1	F	5061	GLN
1	F	5064	GLN
1	F	5070	ARG
1	F	5073	LYS

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Mol	Chain	Res	Type
1	F	5074	LYS
1	F	5075	MSE
1	F	5076	THR
1	F	5077	SER
1	F	5091	ARG
1	F	5098	ARG
1	F	5099	ILE
1	F	5100	LEU
1	F	5106	SER
1	F	5107	LEU
1	F	5108	MSE
1	F	5121	SER
1	F	5123	TYR
1	F	5125	HIS
1	F	5128	ARG
1	F	5136	SER
1	F	5140	ARG
1	F	5152	GLU
1	F	5154	HIS
1	F	5160	VAL
1	F	5179	ILE
1	F	5184	LEU
1	F	5196	ASP
1	F	5203	ILE
1	F	5205	VAL
1	F	5214	LYS
1	F	5219	MSE
1	F	5221	LEU
1	F	5223	GLN
1	F	5224	LYS
1	F	5225	ARG
1	F	5228	THR
1	F	5234	LEU
1	F	5235	ILE
1	F	5248	ARG
1	F	5250	THR
1	F	5251	LEU
1	F	5253	GLN
1	F	5260	HIS
1	F	5261	ASN
1	F	5264	ARG
1	F	5266	LEU

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Mol	Chain	Res	Type
1	F	5267	ARG
1	F	5275	THR
1	F	5276	PHE
1	F	5279	ASP
1	F	5286	VAL
1	F	5291	LEU
1	F	5297	VAL
1	F	5302	ILE
1	F	5304	GLU
1	F	5306	LYS
1	F	5317	LEU
1	F	5329	GLU
1	F	5332	LEU
1	F	5336	GLU
1	F	5338	GLN
1	F	5339	LYS
1	F	5346	LYS
1	F	5349	LEU
1	F	5351	VAL
1	F	5354	ARG
1	F	5355	LYS
1	F	5357	LYS
1	F	5359	ASP
1	F	5366	THR
1	F	5368	SER
1	F	5372	SER
1	F	5376	THR
1	F	5378	GLU
1	F	5383	ILE
1	F	5385	LYS
1	F	5389	ILE
1	F	5397	ARG
1	F	5400	THR
1	F	5402	ASP
1	F	5405	ARG
1	F	5409	SER
1	F	5411	ASN
1	F	5416	ILE
1	F	5419	LEU
1	F	5425	GLN
1	F	5429	THR
1	F	5432	GLU

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Mol	Chain	Res	Type
1	F	5454	LEU
1	F	5456	ASP
1	F	5458	ARG
1	F	5459	VAL
1	F	5479	ILE
1	F	5485	HIS
1	F	5486	ILE
1	F	5487	SER
1	F	5493	GLU
1	F	5496	LYS
1	F	5500	SER
1	F	5502	LEU
1	F	5503	THR
1	F	5504	ASP
1	F	5507	LEU
1	F	5509	GLN
1	F	5511	ARG
1	F	5518	ASN
1	F	5525	ASN
1	F	5533	TYR
1	F	5537	ASN
1	F	5549	LYS
1	F	5551	LYS
1	F	5559	ARG
1	F	5561	GLU
1	F	5565	LEU
1	F	5572	TRP
1	G	6028	LEU
1	G	6029	MSE
1	G	6041	THR
1	G	6043	GLN
1	G	6053	LEU
1	G	6057	LYS
1	G	6071	ASN
1	G	6073	LYS
1	G	6074	LYS
1	G	6075	MSE
1	G	6076	THR
1	G	6077	SER
1	G	6081	LYS
1	G	6086	MSE
1	G	6098	ARG

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Mol	Chain	Res	Type
1	G	6102	ASP
1	G	6104	ILE
1	G	6106	SER
1	G	6108	MSE
1	G	6115	THR
1	G	6123	TYR
1	G	6125	HIS
1	G	6128	ARG
1	G	6131	LYS
1	G	6152	GLU
1	G	6154	HIS
1	G	6156	LYS
1	G	6165	ARG
1	G	6183	LYS
1	G	6184	LEU
1	G	6194	ARG
1	G	6196	ASP
1	G	6205	VAL
1	G	6207	THR
1	G	6210	ILE
1	G	6221	LEU
1	G	6223	GLN
1	G	6224	LYS
1	G	6225	ARG
1	G	6227	ARG
1	G	6232	ASP
1	G	6234	LEU
1	G	6243	THR
1	G	6244	ASP
1	G	6245	ARG
1	G	6250	THR
1	G	6253	GLN
1	G	6264	ARG
1	G	6266	LEU
1	G	6267	ARG
1	G	6268	LYS
1	G	6270	ARG
1	G	6274	CYS
1	G	6276	PHE
1	G	6279	ASP
1	G	6286	VAL
1	G	6291	LEU

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Mol	Chain	Res	Type
1	G	6298	ILE
1	G	6300	LYS
1	G	6304	GLU
1	G	6306	LYS
1	G	6314	GLU
1	G	6317	LEU
1	G	6325	MSE
1	G	6329	GLU
1	G	6332	LEU
1	G	6333	SER
1	G	6334	GLU
1	G	6335	GLN
1	G	6338	GLN
1	G	6341	ILE
1	G	6345	ASP
1	G	6351	VAL
1	G	6355	LYS
1	G	6357	LYS
1	G	6358	ILE
1	G	6363	GLU
1	G	6366	THR
1	G	6371	GLU
1	G	6372	SER
1	G	6378	GLU
1	G	6379	ASP
1	G	6384	LEU
1	G	6385	LYS
1	G	6389	ILE
1	G	6400	THR
1	G	6402	ASP
1	G	6405	ARG
1	G	6412	GLU
1	G	6413	ARG
1	G	6416	ILE
1	G	6419	LEU
1	G	6425	GLN
1	G	6429	THR
1	G	6431	GLU
1	G	6432	GLU
1	G	6438	GLU
1	G	6447	SER
1	G	6454	LEU

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Mol	Chain	Res	Type
1	G	6458	ARG
1	G	6459	VAL
1	G	6467	ASN
1	G	6476	LEU
1	G	6479	ILE
1	G	6482	ASN
1	G	6483	THR
1	G	6486	ILE
1	G	6487	SER
1	G	6489	SER
1	G	6499	THR
1	G	6502	LEU
1	G	6504	ASP
1	G	6505	GLU
1	G	6506	GLU
1	G	6507	LEU
1	G	6509	GLN
1	G	6511	ARG
1	G	6512	LEU
1	G	6518	ASN
1	G	6528	ILE
1	G	6533	TYR
1	G	6535	TYR
1	G	6537	ASN
1	G	6539	MSE
1	G	6549	LYS
1	G	6551	LYS
1	G	6554	LYS
1	G	6559	ARG
1	G	6561	GLU
1	G	6571	GLU
1	G	6572	TRP
1	H	7024	LYS
1	H	7029	MSE
1	H	7030	LEU
1	H	7040	PHE
1	H	7041	THR
1	H	7043	GLN
1	H	7048	LEU
1	H	7057	LYS
1	H	7062	ASP
1	H	7070	ARG

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Mol	Chain	Res	Type
1	H	7075	MSE
1	H	7076	THR
1	H	7082	TYR
1	H	7085	ILE
1	H	7086	MSE
1	H	7098	ARG
1	H	7102	ASP
1	H	7103	ASP
1	H	7108	MSE
1	H	7118	LEU
1	H	7121	SER
1	H	7123	TYR
1	H	7125	HIS
1	H	7128	ARG
1	H	7136	SER
1	H	7145	SER
1	H	7154	HIS
1	H	7160	VAL
1	H	7161	THR
1	H	7175	TYR
1	H	7183	LYS
1	H	7184	LEU
1	H	7185	CYS
1	H	7194	ARG
1	H	7196	ASP
1	H	7199	LEU
1	H	7205	VAL
1	H	7214	LYS
1	H	7223	GLN
1	H	7224	LYS
1	H	7225	ARG
1	H	7228	THR
1	H	7230	GLN
1	H	7232	ASP
1	H	7242	ILE
1	H	7243	THR
1	H	7250	THR
1	H	7253	GLN
1	H	7260	HIS
1	H	7261	ASN
1	H	7264	ARG
1	H	7266	LEU

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Mol	Chain	Res	Type
1	H	7267	ARG
1	H	7270	ARG
1	H	7272	LYS
1	H	7279	ASP
1	H	7283	THR
1	H	7286	VAL
1	H	7292	LEU
1	H	7298	ILE
1	H	7300	LYS
1	H	7304	GLU
1	H	7306	LYS
1	H	7310	LEU
1	H	7319	ILE
1	H	7329	GLU
1	H	7332	LEU
1	H	7333	SER
1	H	7336	GLU
1	H	7341	ILE
1	H	7343	MSE
1	H	7345	ASP
1	H	7346	LYS
1	H	7350	LEU
1	H	7354	ARG
1	H	7359	ASP
1	H	7360	SER
1	H	7368	SER
1	H	7372	SER
1	H	7375	ASP
1	H	7385	LYS
1	H	7389	ILE
1	H	7397	ARG
1	H	7400	THR
1	H	7405	ARG
1	H	7409	SER
1	H	7411	ASN
1	H	7413	ARG
1	H	7415	VAL
1	H	7416	ILE
1	H	7419	LEU
1	H	7425	GLN
1	H	7429	THR
1	H	7431	GLU

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Mol	Chain	Res	Type
1	H	7447	SER
1	H	7453	LYS
1	H	7454	LEU
1	H	7455	THR
1	H	7459	VAL
1	H	7470	ILE
1	H	7479	ILE
1	H	7486	ILE
1	H	7487	SER
1	H	7489	SER
1	H	7492	LEU
1	H	7493	GLU
1	H	7502	LEU
1	H	7507	LEU
1	H	7511	ARG
1	H	7516	LEU
1	H	7518	ASN
1	H	7528	ILE
1	H	7533	TYR
1	H	7539	MSE
1	H	7542	ARG
1	H	7543	TYR
1	H	7549	LYS
1	H	7551	LYS
1	H	7559	ARG
1	H	7561	GLU
1	H	7571	GLU
1	H	7572	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (107) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	GLN
1	A	64	GLN
1	A	71	ASN
1	A	154	HIS
1	A	230	GLN
1	A	253	GLN
1	A	259	ASN
1	A	261	ASN
1	A	295	GLN
1	A	335	GLN

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Mol	Chain	Res	Type
1	A	338	GLN
1	A	411	ASN
1	A	425	GLN
1	A	509	GLN
1	A	520	GLN
1	A	525	ASN
1	B	1064	GLN
1	B	1122	GLN
1	B	1154	HIS
1	B	1229	GLN
1	B	1253	GLN
1	B	1259	ASN
1	B	1261	ASN
1	B	1295	GLN
1	B	1335	GLN
1	B	1411	ASN
1	B	1425	GLN
1	B	1482	ASN
1	B	1509	GLN
1	B	1520	GLN
1	B	1525	ASN
1	B	1537	ASN
1	C	2051	GLN
1	C	2064	GLN
1	C	2253	GLN
1	C	2261	ASN
1	C	2305	HIS
1	C	2338	GLN
1	C	2411	ASN
1	C	2482	ASN
1	C	2537	ASN
1	D	3064	GLN
1	D	3071	ASN
1	D	3122	GLN
1	D	3230	GLN
1	D	3253	GLN
1	D	3261	ASN
1	D	3305	HIS
1	D	3330	ASN
1	D	3335	GLN
1	D	3367	HIS
1	D	3411	ASN

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Mol	Chain	Res	Type
1	D	3425	GLN
1	D	3482	ASN
1	D	3509	GLN
1	D	3525	ASN
1	E	4051	GLN
1	E	4064	GLN
1	E	4071	ASN
1	E	4125	HIS
1	E	4154	HIS
1	E	4223	GLN
1	E	4230	GLN
1	E	4261	ASN
1	E	4295	GLN
1	E	4335	GLN
1	E	4425	GLN
1	E	4482	ASN
1	E	4501	GLN
1	E	4509	GLN
1	E	4525	ASN
1	F	5051	GLN
1	F	5064	GLN
1	F	5223	GLN
1	F	5230	GLN
1	F	5261	ASN
1	F	5335	GLN
1	F	5338	GLN
1	F	5411	ASN
1	F	5425	GLN
1	F	5466	ASN
1	F	5509	GLN
1	F	5525	ASN
1	F	5537	ASN
1	G	6046	GLN
1	G	6064	GLN
1	G	6122	GLN
1	G	6154	HIS
1	G	6230	GLN
1	G	6261	ASN
1	G	6305	HIS
1	G	6335	GLN
1	G	6338	GLN
1	G	6382	ASN

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Mol	Chain	Res	Type
1	G	6425	GLN
1	G	6482	ASN
1	G	6501	GLN
1	H	7064	GLN
1	H	7069	HIS
1	H	7229	GLN
1	H	7261	ASN
1	H	7335	GLN
1	H	7338	GLN
1	H	7411	ASN
1	H	7425	GLN
1	H	7482	ASN
1	H	7537	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 24 ligands modelled in this entry, 8 are monoatomic - leaving 16 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAD	C	2601	-	42,48,48	2.03	11 (26%)	50,73,73	1.42	7 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAD	E	4602	-	42,48,48	2.01	11 (26%)	50,73,73	1.42	6 (12%)
3	NAD	D	3602	-	42,48,48	2.00	10 (23%)	50,73,73	1.49	6 (12%)
3	NAD	F	5602	-	42,48,48	1.98	10 (23%)	50,73,73	1.45	5 (10%)
3	NAD	H	7601	-	42,48,48	2.24	11 (26%)	50,73,73	1.39	6 (12%)
3	NAD	B	1602	-	42,48,48	2.08	9 (21%)	50,73,73	1.41	5 (10%)
3	NAD	G	6602	-	42,48,48	2.02	9 (21%)	50,73,73	1.41	5 (10%)
3	NAD	A	601	-	42,48,48	2.09	12 (28%)	50,73,73	1.49	6 (12%)
3	NAD	A	602	-	42,48,48	2.11	10 (23%)	50,73,73	1.41	4 (8%)
3	NAD	D	3601	-	42,48,48	2.38	14 (33%)	50,73,73	1.48	6 (12%)
3	NAD	F	5601	-	42,48,48	1.94	11 (26%)	50,73,73	1.38	5 (10%)
3	NAD	E	4601	-	42,48,48	2.16	12 (28%)	50,73,73	1.33	4 (8%)
3	NAD	H	7602	-	42,48,48	1.99	9 (21%)	50,73,73	1.48	6 (12%)
3	NAD	B	1601	-	42,48,48	1.97	11 (26%)	50,73,73	1.40	4 (8%)
3	NAD	C	2602	-	42,48,48	2.10	9 (21%)	50,73,73	1.42	6 (12%)
3	NAD	G	6601	-	42,48,48	2.02	11 (26%)	50,73,73	1.49	6 (12%)

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	NAD	C	2601	-	-	5/26/62/62	0/5/5/5
3	NAD	E	4602	-	-	6/26/62/62	0/5/5/5
3	NAD	D	3602	-	-	8/26/62/62	0/5/5/5
3	NAD	F	5602	-	-	6/26/62/62	0/5/5/5
3	NAD	H	7601	-	-	1/26/62/62	0/5/5/5
3	NAD	B	1602	-	-	7/26/62/62	0/5/5/5
3	NAD	G	6602	-	-	7/26/62/62	0/5/5/5
3	NAD	A	601	-	-	1/26/62/62	0/5/5/5
3	NAD	A	602	-	-	6/26/62/62	0/5/5/5
3	NAD	D	3601	-	-	5/26/62/62	0/5/5/5
3	NAD	F	5601	-	-	2/26/62/62	0/5/5/5
3	NAD	E	4601	-	-	2/26/62/62	0/5/5/5
3	NAD	H	7602	-	-	6/26/62/62	0/5/5/5
3	NAD	B	1601	-	-	9/26/62/62	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAD	C	2602	-	-	5/26/62/62	0/5/5/5
3	NAD	G	6601	-	-	1/26/62/62	0/5/5/5

All (170) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1602	NAD	C2N-N1N	8.07	1.44	1.35
3	D	3601	NAD	C2N-N1N	7.62	1.44	1.35
3	C	2602	NAD	C2N-N1N	7.46	1.44	1.35
3	H	7601	NAD	C2N-N1N	7.25	1.43	1.35
3	D	3602	NAD	C2N-N1N	7.16	1.43	1.35
3	F	5602	NAD	C2N-N1N	7.02	1.43	1.35
3	A	602	NAD	C2N-N1N	7.00	1.43	1.35
3	G	6602	NAD	C2N-N1N	6.99	1.43	1.35
3	H	7602	NAD	C2N-N1N	6.91	1.43	1.35
3	A	601	NAD	C2N-N1N	6.77	1.43	1.35
3	E	4601	NAD	C2N-N1N	6.70	1.43	1.35
3	C	2601	NAD	C2N-N1N	6.69	1.43	1.35
3	E	4602	NAD	C2N-N1N	6.65	1.43	1.35
3	G	6601	NAD	C2N-N1N	6.18	1.42	1.35
3	H	7601	NAD	O4B-C1B	6.03	1.49	1.41
3	D	3601	NAD	O4D-C1D	5.99	1.49	1.41
3	B	1601	NAD	C2N-N1N	5.82	1.42	1.35
3	A	601	NAD	O4D-C1D	5.27	1.48	1.41
3	F	5601	NAD	C2N-N1N	5.22	1.41	1.35
3	E	4601	NAD	O4D-C1D	5.18	1.48	1.41
3	A	602	NAD	O4B-C1B	5.04	1.48	1.41
3	C	2602	NAD	O4B-C1B	4.93	1.48	1.41
3	C	2602	NAD	O4D-C1D	4.74	1.47	1.41
3	D	3601	NAD	C3N-C7N	4.69	1.57	1.50
3	B	1601	NAD	O4D-C1D	4.68	1.47	1.41
3	F	5601	NAD	O4B-C1B	4.58	1.47	1.41
3	E	4601	NAD	O4B-C1B	4.56	1.47	1.41
3	D	3601	NAD	O4B-C1B	4.43	1.47	1.41
3	D	3602	NAD	O4D-C1D	4.40	1.47	1.41
3	B	1601	NAD	O4B-C1B	4.36	1.47	1.41
3	A	602	NAD	O4D-C1D	4.32	1.47	1.41
3	G	6602	NAD	O4B-C1B	4.30	1.47	1.41
3	F	5602	NAD	O4B-C1B	4.30	1.47	1.41
3	H	7601	NAD	O4D-C1D	4.26	1.47	1.41
3	G	6601	NAD	C3N-C7N	4.22	1.56	1.50
3	H	7601	NAD	C2A-N3A	4.18	1.38	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	7602	NAD	O4B-C1B	4.16	1.46	1.41
3	F	5602	NAD	O4D-C1D	4.15	1.46	1.41
3	E	4602	NAD	O4D-C1D	4.13	1.46	1.41
3	D	3602	NAD	O4B-C1B	4.10	1.46	1.41
3	H	7602	NAD	O4D-C1D	4.07	1.46	1.41
3	D	3601	NAD	C2A-N3A	4.07	1.38	1.32
3	G	6602	NAD	O4D-C1D	4.05	1.46	1.41
3	D	3601	NAD	C6N-N1N	4.01	1.45	1.35
3	B	1602	NAD	O4D-C1D	4.01	1.46	1.41
3	E	4602	NAD	C6N-N1N	3.99	1.45	1.35
3	A	601	NAD	C6N-N1N	3.97	1.45	1.35
3	E	4602	NAD	O4B-C1B	3.94	1.46	1.41
3	C	2601	NAD	O4D-C1D	3.92	1.46	1.41
3	C	2601	NAD	C6N-N1N	3.91	1.45	1.35
3	F	5601	NAD	C2D-C1D	-3.91	1.47	1.53
3	A	601	NAD	C3N-C7N	3.89	1.56	1.50
3	E	4601	NAD	C2D-C1D	-3.89	1.47	1.53
3	H	7602	NAD	C6N-N1N	3.88	1.44	1.35
3	G	6601	NAD	C2A-N3A	3.87	1.38	1.32
3	A	602	NAD	C6N-N1N	3.84	1.44	1.35
3	F	5602	NAD	C6N-N1N	3.83	1.44	1.35
3	G	6602	NAD	C6N-N1N	3.82	1.44	1.35
3	B	1602	NAD	C6N-N1N	3.80	1.44	1.35
3	D	3602	NAD	C6N-N1N	3.78	1.44	1.35
3	F	5601	NAD	C6N-N1N	3.74	1.44	1.35
3	C	2602	NAD	C6N-N1N	3.74	1.44	1.35
3	B	1601	NAD	C2A-N3A	3.73	1.38	1.32
3	C	2601	NAD	C2B-C1B	-3.72	1.48	1.53
3	B	1602	NAD	C2A-N3A	3.63	1.37	1.32
3	E	4601	NAD	C6N-N1N	3.63	1.44	1.35
3	C	2601	NAD	C2A-N3A	3.60	1.37	1.32
3	F	5601	NAD	C2A-N3A	3.59	1.37	1.32
3	G	6602	NAD	C2A-N3A	3.58	1.37	1.32
3	B	1602	NAD	O4B-C1B	3.56	1.46	1.41
3	E	4601	NAD	C2A-N3A	3.54	1.37	1.32
3	H	7601	NAD	C3N-C7N	3.53	1.55	1.50
3	A	602	NAD	C2A-N3A	3.52	1.37	1.32
3	G	6601	NAD	O4B-C1B	3.48	1.45	1.41
3	G	6601	NAD	C6N-N1N	3.47	1.43	1.35
3	A	601	NAD	O4B-C1B	3.38	1.45	1.41
3	C	2602	NAD	C3N-C7N	3.36	1.55	1.50
3	A	601	NAD	C2A-N3A	3.36	1.37	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	4602	NAD	C2A-N3A	3.34	1.37	1.32
3	H	7602	NAD	C2A-N3A	3.33	1.37	1.32
3	C	2601	NAD	C3N-C7N	3.29	1.55	1.50
3	G	6601	NAD	O4D-C1D	3.29	1.45	1.41
3	A	602	NAD	C3N-C7N	3.27	1.55	1.50
3	F	5602	NAD	C3N-C7N	3.25	1.55	1.50
3	G	6601	NAD	C2D-C1D	-3.24	1.48	1.53
3	G	6602	NAD	C3N-C7N	3.22	1.55	1.50
3	D	3602	NAD	C3N-C7N	3.21	1.55	1.50
3	B	1601	NAD	C3N-C7N	3.20	1.55	1.50
3	H	7601	NAD	C6N-N1N	3.20	1.43	1.35
3	H	7602	NAD	C3N-C7N	3.18	1.55	1.50
3	E	4601	NAD	C3N-C7N	3.14	1.55	1.50
3	F	5601	NAD	C3N-C7N	3.09	1.55	1.50
3	E	4602	NAD	C3N-C7N	3.05	1.55	1.50
3	C	2602	NAD	C2A-N3A	3.05	1.37	1.32
3	C	2601	NAD	C5A-C4A	-3.02	1.32	1.40
3	B	1601	NAD	C6N-N1N	2.99	1.42	1.35
3	C	2601	NAD	O4B-C1B	2.94	1.45	1.41
3	D	3601	NAD	C4N-C3N	2.92	1.44	1.39
3	D	3601	NAD	C2N-C3N	2.87	1.43	1.39
3	F	5601	NAD	C4N-C3N	2.85	1.44	1.39
3	B	1602	NAD	C3N-C7N	2.85	1.54	1.50
3	F	5601	NAD	C5A-C4A	-2.85	1.33	1.40
3	A	601	NAD	C5A-C4A	-2.85	1.33	1.40
3	B	1602	NAD	C5A-C4A	-2.84	1.33	1.40
3	F	5602	NAD	C2A-N3A	2.82	1.36	1.32
3	E	4602	NAD	C2B-C1B	-2.79	1.49	1.53
3	E	4602	NAD	C5A-C4A	-2.77	1.33	1.40
3	C	2602	NAD	C5A-C4A	-2.73	1.33	1.40
3	H	7601	NAD	C5A-C4A	-2.73	1.33	1.40
3	F	5602	NAD	C5A-C4A	-2.73	1.33	1.40
3	C	2601	NAD	C2D-C1D	-2.72	1.49	1.53
3	G	6602	NAD	C5A-C4A	-2.69	1.33	1.40
3	E	4601	NAD	C5A-C4A	-2.68	1.33	1.40
3	G	6601	NAD	C5A-C4A	-2.64	1.33	1.40
3	D	3601	NAD	C5A-C4A	-2.61	1.34	1.40
3	A	602	NAD	C2A-N1A	2.60	1.38	1.33
3	H	7601	NAD	C2B-C1B	-2.58	1.49	1.53
3	D	3601	NAD	C5A-N7A	-2.57	1.30	1.39
3	G	6601	NAD	C5A-N7A	-2.57	1.30	1.39
3	E	4602	NAD	C5A-N7A	-2.57	1.30	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602	NAD	C5A-N7A	-2.52	1.30	1.39
3	H	7602	NAD	C5A-C4A	-2.51	1.34	1.40
3	A	601	NAD	C2D-C1D	-2.50	1.50	1.53
3	A	601	NAD	C5A-N7A	-2.49	1.30	1.39
3	B	1601	NAD	C2A-N1A	2.44	1.38	1.33
3	A	602	NAD	C5A-C4A	-2.43	1.34	1.40
3	G	6601	NAD	C4N-C3N	2.43	1.43	1.39
3	D	3602	NAD	C5A-C4A	-2.43	1.34	1.40
3	B	1601	NAD	C4A-N3A	2.41	1.39	1.35
3	D	3602	NAD	C2A-N3A	2.41	1.36	1.32
3	B	1601	NAD	C5A-C4A	-2.38	1.34	1.40
3	G	6601	NAD	C2A-N1A	2.38	1.38	1.33
3	C	2601	NAD	C5A-N7A	-2.37	1.31	1.39
3	F	5601	NAD	C5A-N7A	-2.37	1.31	1.39
3	D	3602	NAD	C2A-N1A	2.36	1.38	1.33
3	H	7601	NAD	C5A-N7A	-2.35	1.31	1.39
3	D	3601	NAD	PN-O5D	2.34	1.68	1.59
3	E	4601	NAD	C4N-C3N	2.33	1.43	1.39
3	F	5601	NAD	O4D-C1D	2.33	1.44	1.41
3	A	601	NAD	C2A-N1A	2.29	1.38	1.33
3	E	4602	NAD	C4N-C3N	2.26	1.43	1.39
3	C	2602	NAD	C5A-N7A	-2.26	1.31	1.39
3	B	1602	NAD	C5A-N7A	-2.24	1.31	1.39
3	G	6602	NAD	C5A-N7A	-2.24	1.31	1.39
3	H	7602	NAD	C5A-N7A	-2.23	1.31	1.39
3	A	601	NAD	C2B-C1B	-2.22	1.50	1.53
3	E	4601	NAD	C2A-N1A	2.22	1.38	1.33
3	E	4601	NAD	C5A-N7A	-2.19	1.31	1.39
3	F	5602	NAD	C4N-C3N	2.19	1.43	1.39
3	G	6602	NAD	C4N-C3N	2.19	1.43	1.39
3	C	2602	NAD	C4N-C3N	2.18	1.43	1.39
3	B	1601	NAD	C5A-N7A	-2.17	1.31	1.39
3	H	7602	NAD	C4N-C3N	2.17	1.43	1.39
3	D	3602	NAD	C4N-C3N	2.16	1.43	1.39
3	H	7601	NAD	C2A-N1A	2.15	1.37	1.33
3	A	602	NAD	C4N-C3N	2.15	1.43	1.39
3	C	2601	NAD	C4N-C3N	2.12	1.42	1.39
3	B	1602	NAD	C2N-C3N	2.10	1.42	1.39
3	F	5601	NAD	C2A-N1A	2.10	1.37	1.33
3	D	3602	NAD	C5A-N7A	-2.09	1.32	1.39
3	A	601	NAD	C2N-C3N	2.08	1.42	1.39
3	B	1601	NAD	O4D-C4D	2.08	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	5602	NAD	C5A-N7A	-2.07	1.32	1.39
3	E	4602	NAD	C2A-N1A	2.07	1.37	1.33
3	F	5602	NAD	C2A-N1A	2.07	1.37	1.33
3	D	3601	NAD	C2A-N1A	2.03	1.37	1.33
3	D	3601	NAD	C5D-C4D	2.02	1.57	1.51
3	H	7601	NAD	C2D-C1D	-2.01	1.50	1.53
3	E	4601	NAD	C5N-C4N	2.01	1.43	1.38
3	D	3601	NAD	C2D-C1D	-2.01	1.50	1.53

All (87) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	5601	NAD	N3A-C2A-N1A	-5.44	120.17	128.68
3	E	4601	NAD	N3A-C2A-N1A	-5.36	120.30	128.68
3	G	6601	NAD	N3A-C2A-N1A	-5.36	120.30	128.68
3	C	2601	NAD	N3A-C2A-N1A	-5.34	120.33	128.68
3	A	601	NAD	N3A-C2A-N1A	-5.31	120.37	128.68
3	B	1601	NAD	N3A-C2A-N1A	-5.29	120.41	128.68
3	F	5602	NAD	N3A-C2A-N1A	-5.15	120.64	128.68
3	B	1602	NAD	N3A-C2A-N1A	-5.14	120.64	128.68
3	H	7601	NAD	N3A-C2A-N1A	-5.14	120.65	128.68
3	C	2602	NAD	N3A-C2A-N1A	-5.06	120.77	128.68
3	E	4602	NAD	N3A-C2A-N1A	-5.06	120.78	128.68
3	A	602	NAD	N3A-C2A-N1A	-5.03	120.81	128.68
3	D	3602	NAD	N3A-C2A-N1A	-5.00	120.86	128.68
3	D	3601	NAD	N3A-C2A-N1A	-5.00	120.86	128.68
3	G	6602	NAD	N3A-C2A-N1A	-5.00	120.86	128.68
3	H	7602	NAD	N3A-C2A-N1A	-4.90	121.02	128.68
3	F	5601	NAD	C4A-C5A-N7A	4.47	114.06	109.40
3	E	4601	NAD	C4A-C5A-N7A	4.42	114.00	109.40
3	A	601	NAD	C4A-C5A-N7A	4.39	113.98	109.40
3	G	6601	NAD	C4A-C5A-N7A	4.39	113.97	109.40
3	B	1601	NAD	C4A-C5A-N7A	4.34	113.93	109.40
3	C	2601	NAD	C4A-C5A-N7A	4.34	113.92	109.40
3	D	3601	NAD	C4A-C5A-N7A	4.27	113.84	109.40
3	H	7602	NAD	C4A-C5A-N7A	4.23	113.81	109.40
3	D	3602	NAD	C4A-C5A-N7A	4.22	113.79	109.40
3	E	4602	NAD	C4A-C5A-N7A	4.21	113.78	109.40
3	H	7601	NAD	C4A-C5A-N7A	4.20	113.78	109.40
3	F	5602	NAD	C4A-C5A-N7A	4.20	113.78	109.40
3	A	602	NAD	C4A-C5A-N7A	4.20	113.77	109.40
3	C	2602	NAD	C4A-C5A-N7A	4.17	113.75	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1602	NAD	C4A-C5A-N7A	4.10	113.67	109.40
3	G	6602	NAD	C4A-C5A-N7A	4.03	113.60	109.40
3	A	601	NAD	C3D-C2D-C1D	3.84	106.76	100.98
3	H	7602	NAD	C3B-C2B-C1B	3.81	106.71	100.98
3	E	4602	NAD	C3D-C2D-C1D	3.63	106.44	100.98
3	F	5602	NAD	C3D-C2D-C1D	3.60	106.40	100.98
3	D	3602	NAD	C3D-C2D-C1D	3.57	106.36	100.98
3	G	6601	NAD	C3B-C2B-C1B	3.56	106.33	100.98
3	H	7602	NAD	C3D-C2D-C1D	3.55	106.32	100.98
3	D	3601	NAD	C3B-C2B-C1B	3.55	106.32	100.98
3	A	602	NAD	C3D-C2D-C1D	3.52	106.27	100.98
3	B	1602	NAD	C3D-C2D-C1D	3.51	106.26	100.98
3	G	6602	NAD	C3D-C2D-C1D	3.50	106.24	100.98
3	C	2602	NAD	C3D-C2D-C1D	3.48	106.22	100.98
3	D	3601	NAD	C3D-C2D-C1D	3.47	106.20	100.98
3	G	6601	NAD	C3D-C2D-C1D	3.45	106.17	100.98
3	D	3602	NAD	C3B-C2B-C1B	3.44	106.16	100.98
3	C	2601	NAD	C3D-C2D-C1D	3.29	105.93	100.98
3	H	7601	NAD	C3D-C2D-C1D	3.20	105.80	100.98
3	A	601	NAD	C3B-C2B-C1B	3.14	105.70	100.98
3	B	1601	NAD	C3D-C2D-C1D	3.06	105.59	100.98
3	F	5602	NAD	C3B-C2B-C1B	2.93	105.38	100.98
3	B	1601	NAD	C3B-C2B-C1B	2.72	105.07	100.98
3	F	5601	NAD	C3D-C2D-C1D	2.70	105.04	100.98
3	H	7601	NAD	C3B-C2B-C1B	2.66	104.98	100.98
3	C	2601	NAD	C3B-C2B-C1B	2.65	104.96	100.98
3	A	601	NAD	C6N-N1N-C2N	-2.61	119.59	121.97
3	C	2602	NAD	C6N-N1N-C2N	-2.57	119.63	121.97
3	E	4602	NAD	C6N-N1N-C2N	-2.56	119.64	121.97
3	D	3602	NAD	C6N-N1N-C2N	-2.55	119.65	121.97
3	F	5602	NAD	C6N-N1N-C2N	-2.55	119.65	121.97
3	D	3601	NAD	C6N-N1N-C2N	-2.54	119.66	121.97
3	B	1602	NAD	C6N-N1N-C2N	-2.53	119.67	121.97
3	H	7602	NAD	C6N-N1N-C2N	-2.48	119.71	121.97
3	A	602	NAD	C6N-N1N-C2N	-2.46	119.73	121.97
3	G	6602	NAD	C6N-N1N-C2N	-2.46	119.73	121.97
3	G	6602	NAD	C3B-C2B-C1B	2.45	104.67	100.98
3	B	1602	NAD	C3B-C2B-C1B	2.42	104.63	100.98
3	H	7601	NAD	C6N-N1N-C2N	-2.39	119.80	121.97
3	C	2602	NAD	C3B-C2B-C1B	2.35	104.52	100.98
3	E	4601	NAD	C3D-C2D-C1D	2.32	104.48	100.98
3	E	4601	NAD	C3B-C2B-C1B	2.32	104.47	100.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	6601	NAD	C6N-N1N-C2N	-2.26	119.91	121.97
3	E	4602	NAD	C3B-C2B-C1B	2.24	104.36	100.98
3	G	6601	NAD	C2B-C3B-C4B	2.20	106.92	102.64
3	D	3601	NAD	C2D-C3D-C4D	2.14	106.81	102.64
3	F	5601	NAD	C3B-C2B-C1B	2.13	104.19	100.98
3	F	5601	NAD	C3N-C7N-N7N	-2.12	115.21	117.75
3	A	601	NAD	C3N-C7N-N7N	-2.11	115.22	117.75
3	C	2601	NAD	C3N-C7N-N7N	-2.09	115.24	117.75
3	C	2601	NAD	C2D-C3D-C4D	2.09	106.70	102.64
3	H	7601	NAD	C3N-C7N-N7N	-2.05	115.29	117.75
3	E	4602	NAD	C2D-C3D-C4D	2.05	106.63	102.64
3	H	7602	NAD	C2B-C3B-C4B	2.03	106.59	102.64
3	D	3602	NAD	C2D-C3D-C4D	2.03	106.59	102.64
3	C	2602	NAD	C2D-C3D-C4D	2.03	106.59	102.64
3	C	2601	NAD	C6N-N1N-C2N	-2.02	120.13	121.97

There are no chirality outliers.

All (77) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	602	NAD	C5B-O5B-PA-O1A
3	F	5601	NAD	PN-O3-PA-O5B
3	E	4602	NAD	C5B-O5B-PA-O1A
3	E	4602	NAD	C5D-O5D-PN-O1N
3	E	4602	NAD	C3D-C4D-C5D-O5D
3	D	3602	NAD	C5B-O5B-PA-O1A
3	D	3602	NAD	C5B-O5B-PA-O2A
3	D	3602	NAD	C3D-C4D-C5D-O5D
3	G	6602	NAD	C5B-O5B-PA-O1A
3	G	6602	NAD	C5B-O5B-PA-O2A
3	G	6602	NAD	C3D-C4D-C5D-O5D
3	C	2601	NAD	C5B-O5B-PA-O1A
3	C	2601	NAD	O4B-C4B-C5B-O5B
3	C	2601	NAD	C3B-C4B-C5B-O5B
3	E	4601	NAD	PN-O3-PA-O5B
3	B	1601	NAD	C5B-O5B-PA-O1A
3	B	1601	NAD	C5B-O5B-PA-O2A
3	F	5602	NAD	C5B-O5B-PA-O1A
3	F	5602	NAD	C5D-O5D-PN-O1N
3	H	7602	NAD	C5B-O5B-PA-O1A
3	H	7602	NAD	C5B-O5B-PA-O2A
3	D	3601	NAD	C5D-O5D-PN-O3

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Mol	Chain	Res	Type	Atoms
3	B	1602	NAD	C5B-O5B-PA-O1A
3	B	1602	NAD	C5D-O5D-PN-O1N
3	B	1602	NAD	C3D-C4D-C5D-O5D
3	C	2602	NAD	C5B-O5B-PA-O2A
3	C	2602	NAD	C5B-O5B-PA-O3
3	C	2602	NAD	C5D-O5D-PN-O1N
3	B	1601	NAD	O4B-C4B-C5B-O5B
3	B	1601	NAD	C3B-C4B-C5B-O5B
3	H	7602	NAD	C3D-C4D-C5D-O5D
3	D	3601	NAD	O4D-C4D-C5D-O5D
3	D	3602	NAD	O4D-C4D-C5D-O5D
3	D	3601	NAD	C3D-C4D-C5D-O5D
3	B	1602	NAD	O4D-C4D-C5D-O5D
3	E	4602	NAD	O4D-C4D-C5D-O5D
3	G	6602	NAD	O4D-C4D-C5D-O5D
3	H	7602	NAD	O4D-C4D-C5D-O5D
3	A	602	NAD	C3D-C4D-C5D-O5D
3	B	1601	NAD	PN-O3-PA-O5B
3	E	4602	NAD	C5B-O5B-PA-O3
3	C	2601	NAD	C5B-O5B-PA-O3
3	A	602	NAD	C5B-O5B-PA-O2A
3	E	4602	NAD	C5B-O5B-PA-O2A
3	D	3602	NAD	C5D-O5D-PN-O2N
3	C	2601	NAD	C5B-O5B-PA-O2A
3	F	5602	NAD	C5B-O5B-PA-O2A
3	B	1602	NAD	C5B-O5B-PA-O2A
3	B	1601	NAD	O4D-C4D-C5D-O5D
3	C	2602	NAD	C3D-C4D-C5D-O5D
3	G	6602	NAD	C4B-C5B-O5B-PA
3	H	7601	NAD	O4B-C4B-C5B-O5B
3	F	5602	NAD	C3D-C4D-C5D-O5D
3	B	1601	NAD	PA-O3-PN-O2N
3	A	602	NAD	O4B-C4B-C5B-O5B
3	D	3602	NAD	O4B-C4B-C5B-O5B
3	A	602	NAD	C5B-O5B-PA-O3
3	D	3602	NAD	C5B-O5B-PA-O3
3	D	3602	NAD	C5D-O5D-PN-O3
3	G	6602	NAD	C5B-O5B-PA-O3
3	B	1601	NAD	C5B-O5B-PA-O3
3	F	5602	NAD	C5B-O5B-PA-O3
3	F	5602	NAD	C5D-O5D-PN-O3
3	H	7602	NAD	C5B-O5B-PA-O3

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Mol	Chain	Res	Type	Atoms
3	B	1602	NAD	C5B-O5B-PA-O3
3	C	2602	NAD	C5D-O5D-PN-O3
3	A	601	NAD	O4B-C4B-C5B-O5B
3	E	4601	NAD	O4B-C4B-C5B-O5B
3	G	6601	NAD	O4B-C4B-C5B-O5B
3	H	7602	NAD	PN-O3-PA-O2A
3	B	1602	NAD	C4B-C5B-O5B-PA
3	G	6602	NAD	C5D-O5D-PN-O1N
3	D	3601	NAD	C5D-O5D-PN-O1N
3	A	602	NAD	C3B-C4B-C5B-O5B
3	F	5601	NAD	O4B-C4B-C5B-O5B
3	B	1601	NAD	C3D-C4D-C5D-O5D
3	D	3601	NAD	O4B-C4B-C5B-O5B

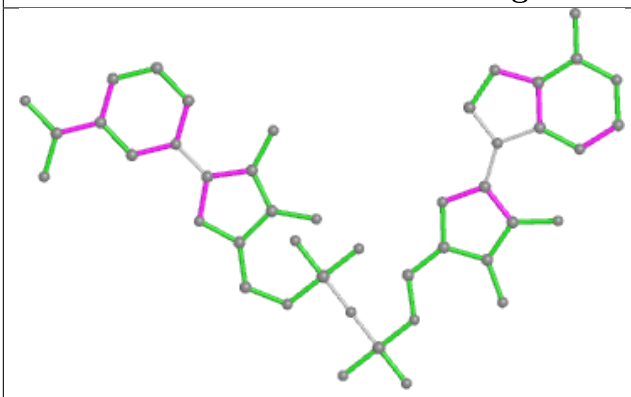
There are no ring outliers.

11 monomers are involved in 27 short contacts:

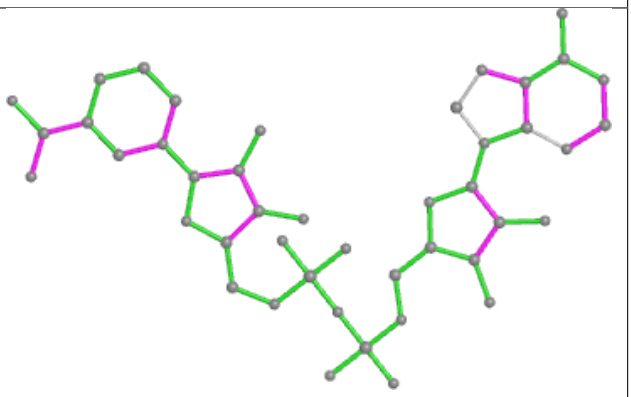
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	2601	NAD	2	0
3	D	3602	NAD	1	0
3	H	7601	NAD	2	0
3	B	1602	NAD	1	0
3	A	601	NAD	3	0
3	D	3601	NAD	3	0
3	F	5601	NAD	3	0
3	E	4601	NAD	3	0
3	H	7602	NAD	1	0
3	B	1601	NAD	4	0
3	G	6601	NAD	4	0

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

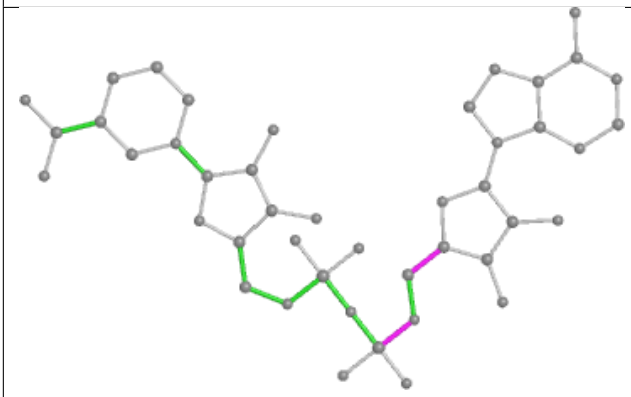
Ligand NAD C 2601



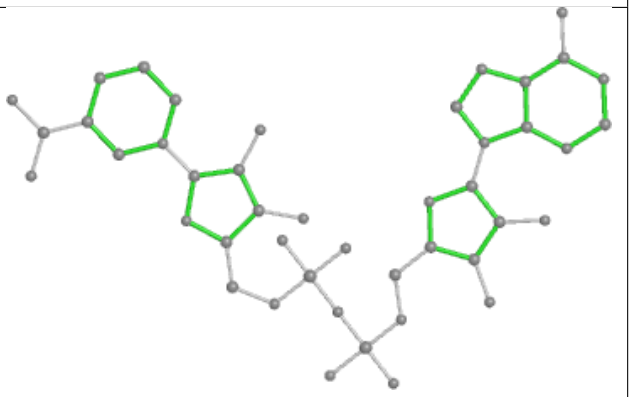
Bond lengths



Bond angles

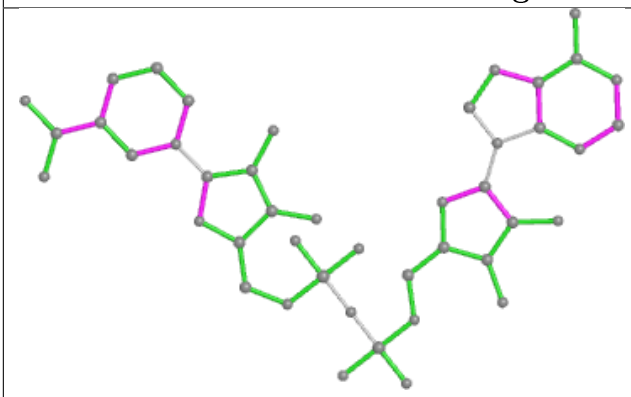


Torsions



Rings

Ligand NAD E 4602



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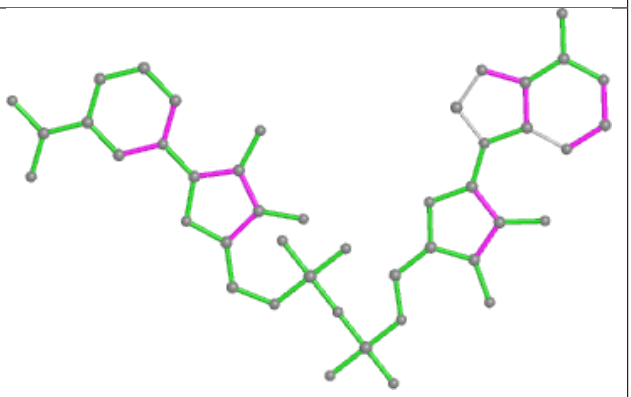

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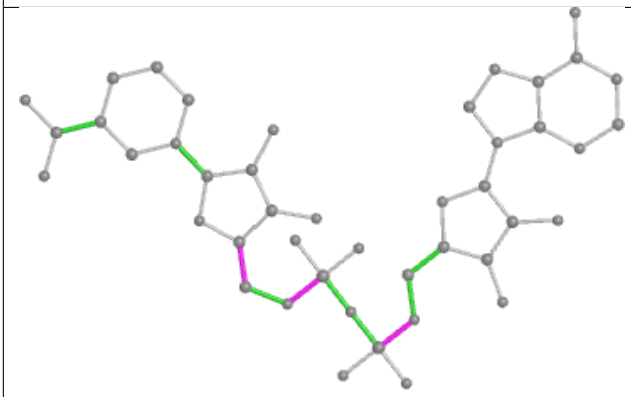

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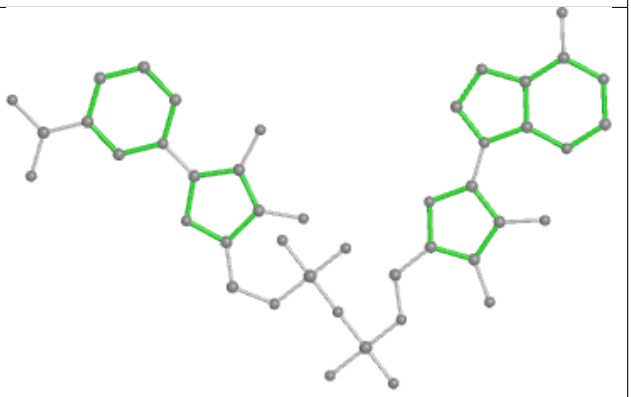
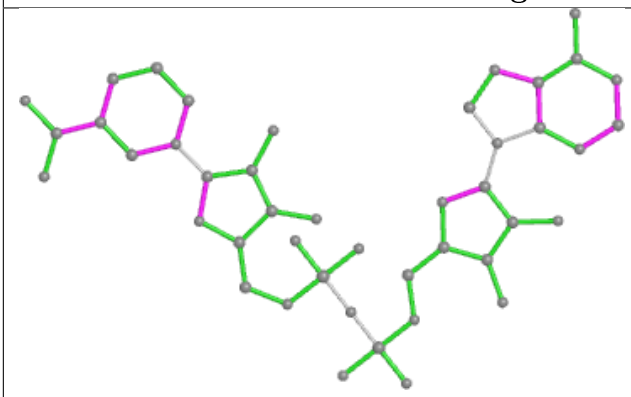
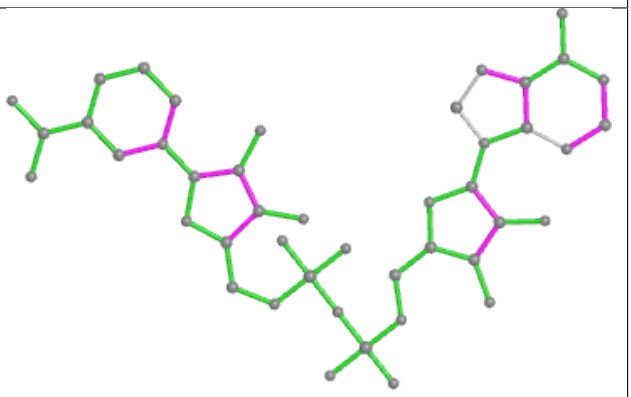


Rings

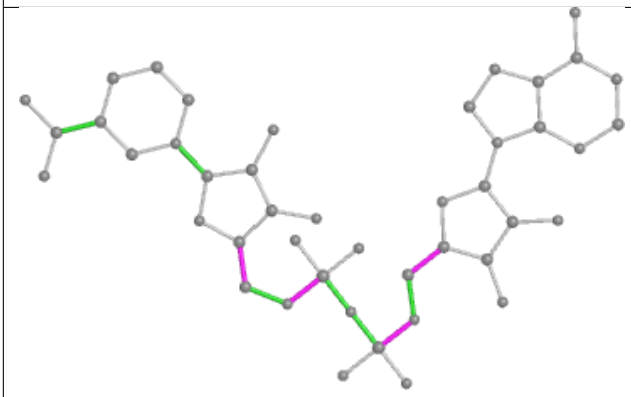
Ligand NAD D 3602



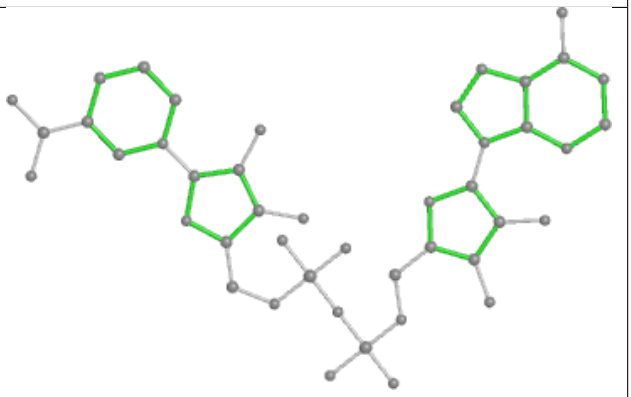
Bond lengths



Bond angles

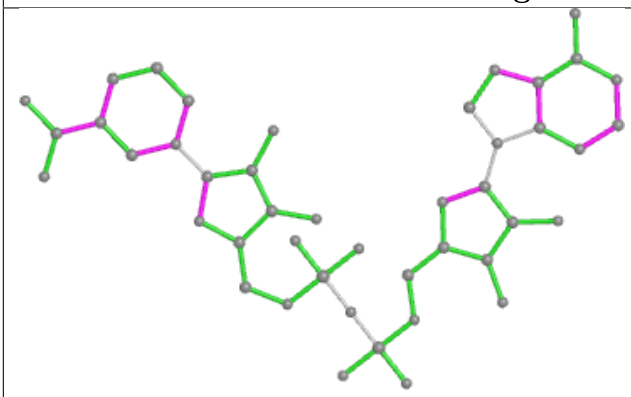


Torsions

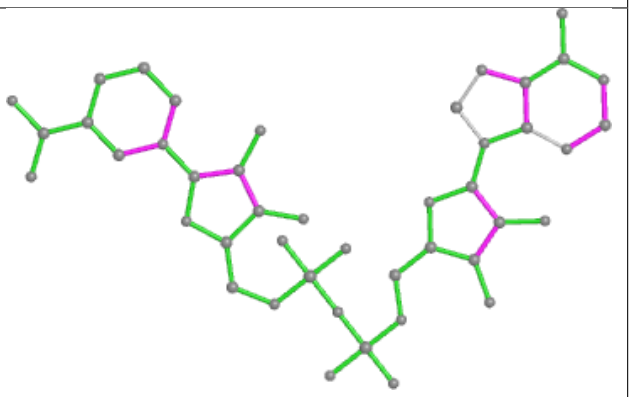


Rings

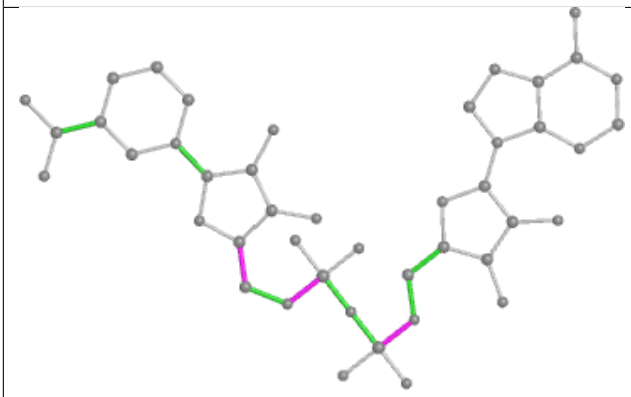
Ligand NAD F 5602



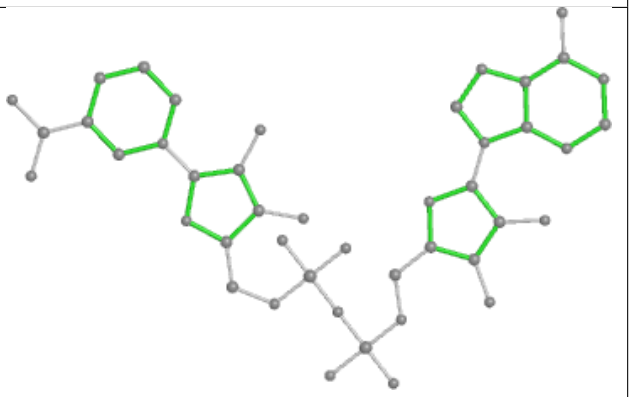
Bond lengths



Bond angles

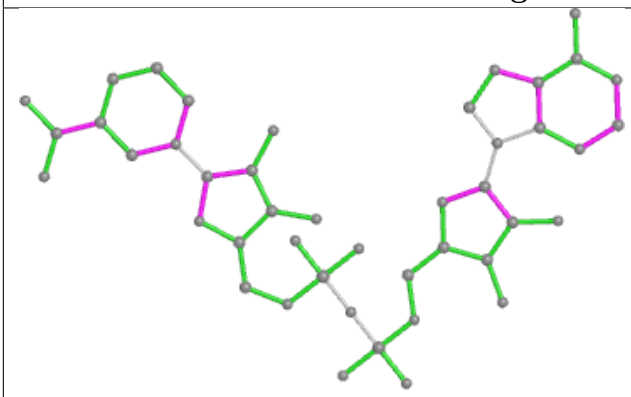


Torsions

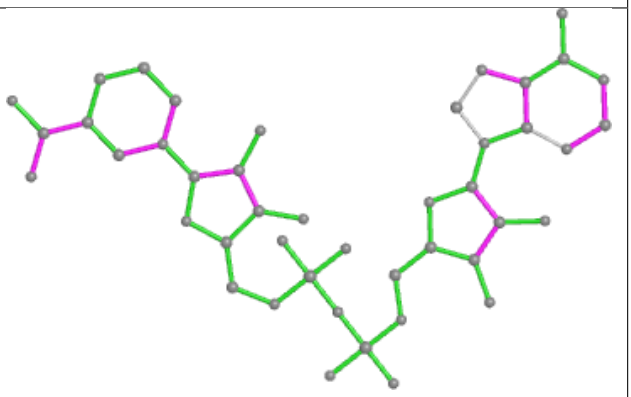


Rings

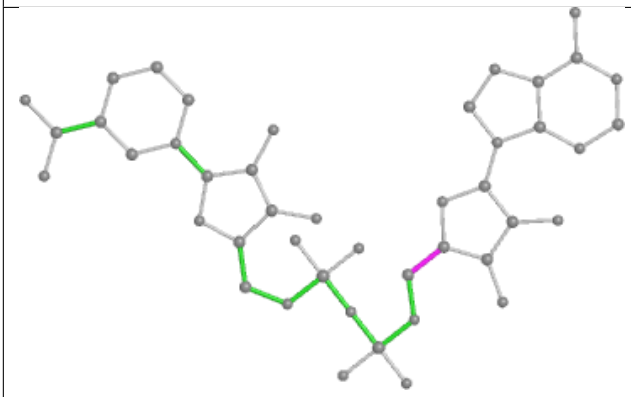
Ligand NAD H 7601



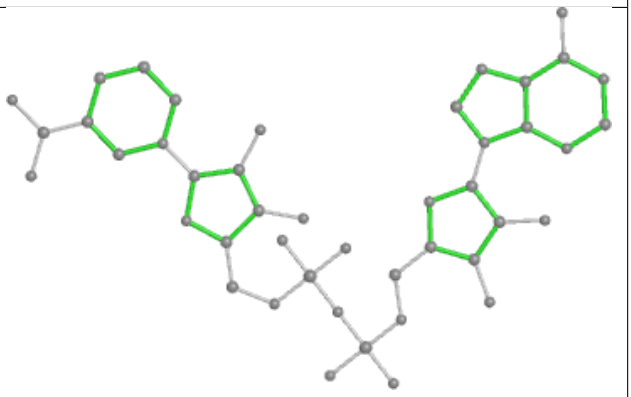
Bond lengths



Bond angles

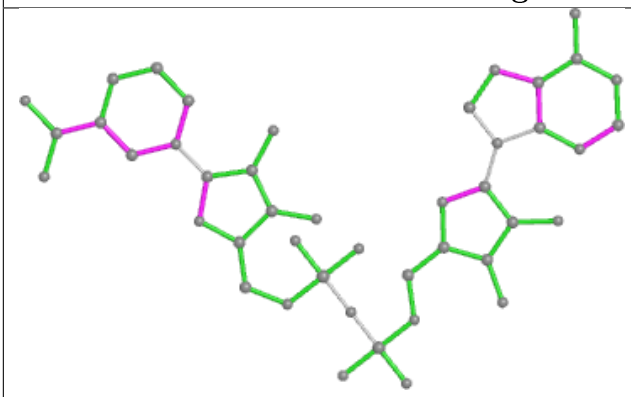


Torsions



Rings

Ligand NAD B 1602



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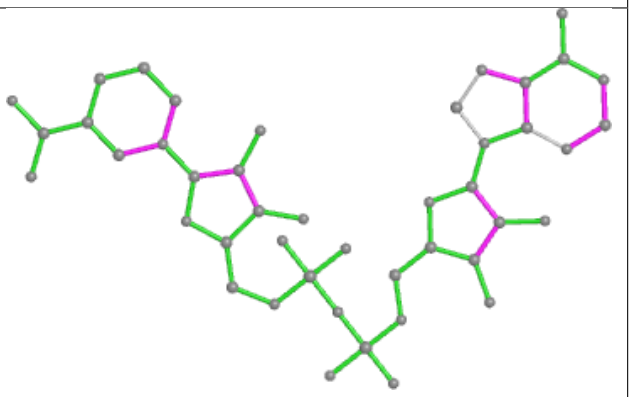

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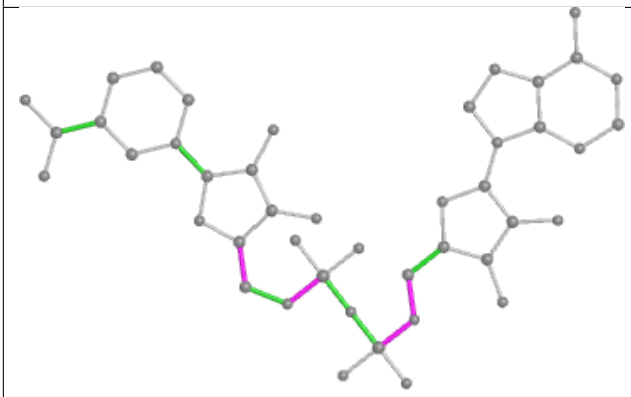

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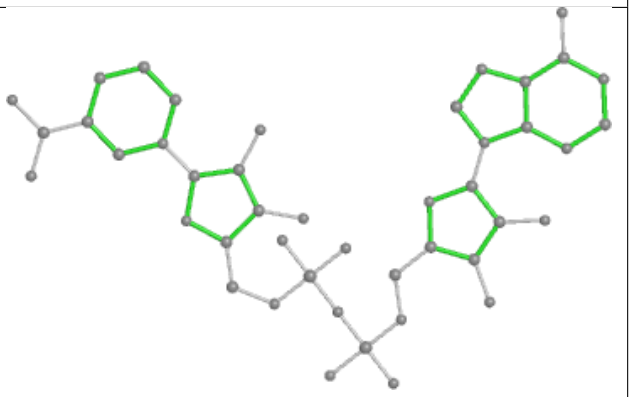
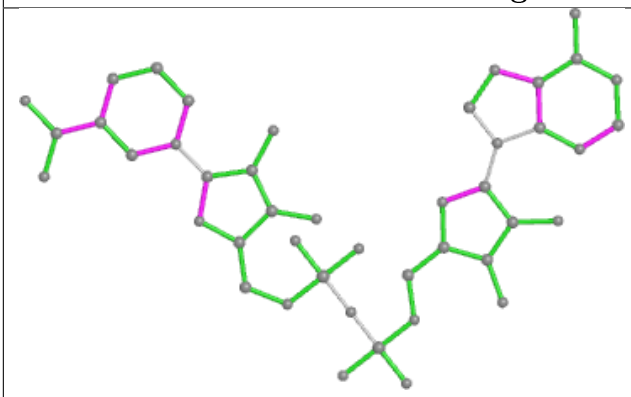
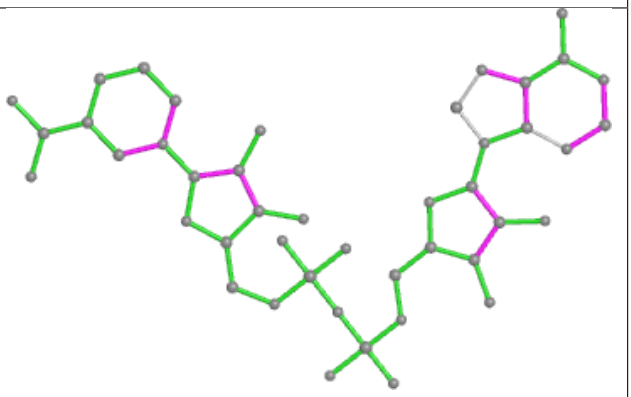


Rings

Ligand NAD G 6602



Bond lengths



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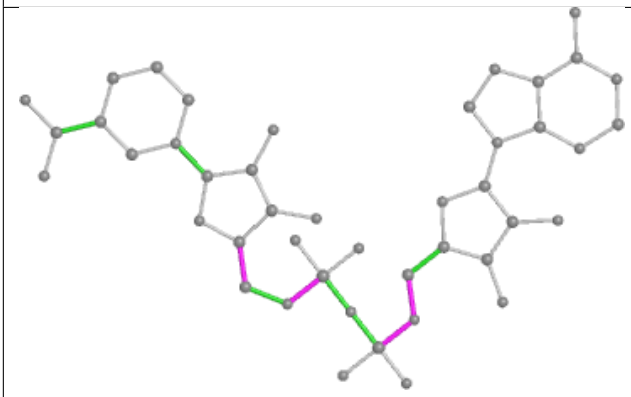

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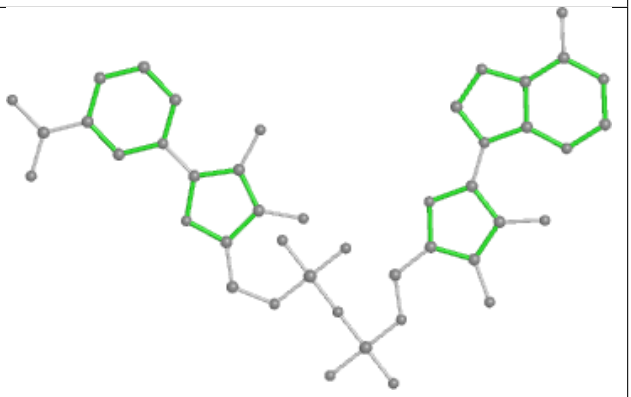
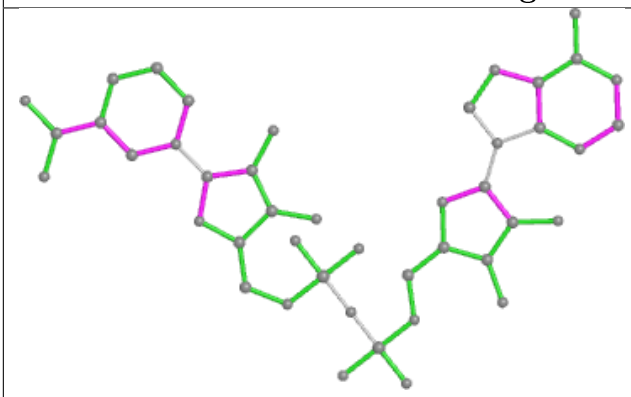


Rings

Ligand NAD A 601



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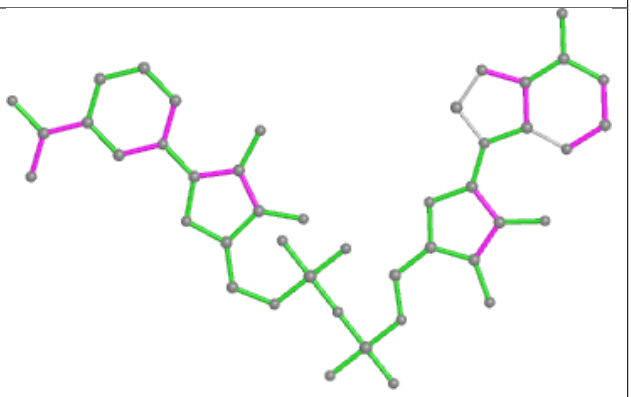

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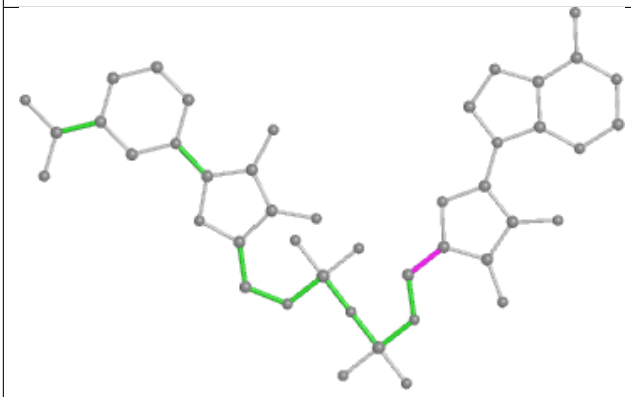
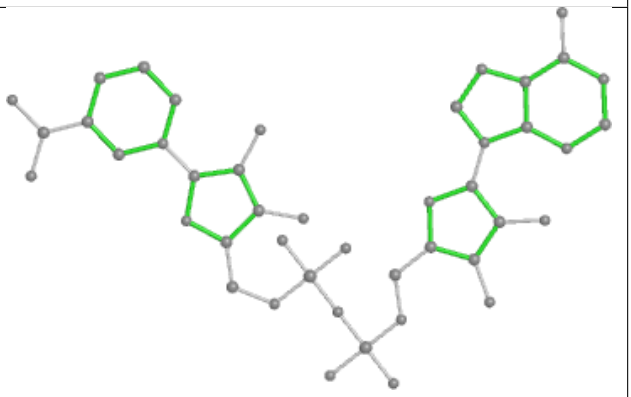
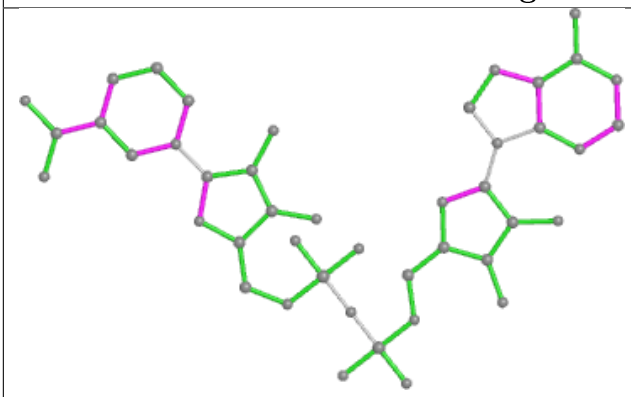


Torsions

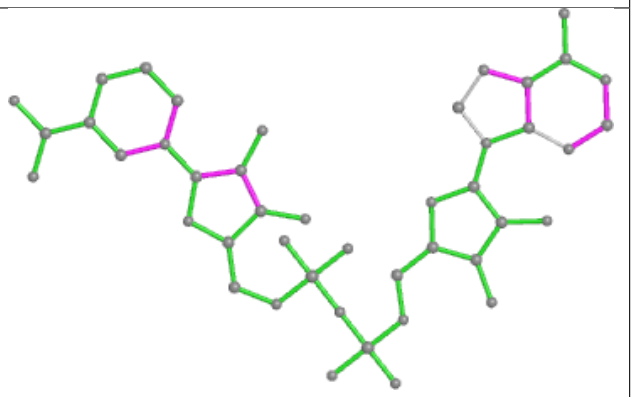


Rings

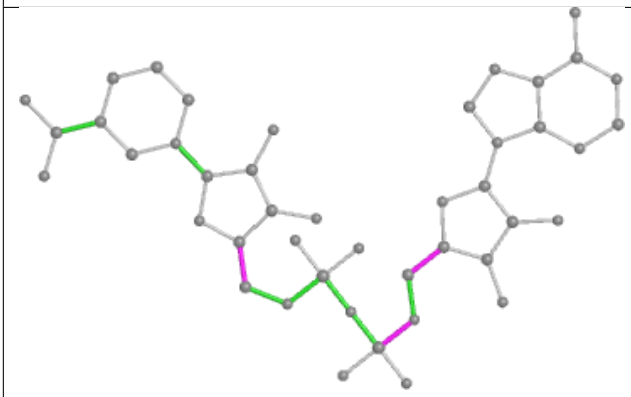
Ligand NAD A 602



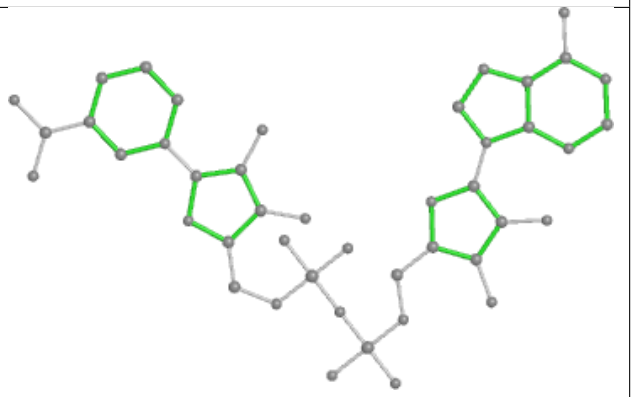
Bond lengths



Bond angles

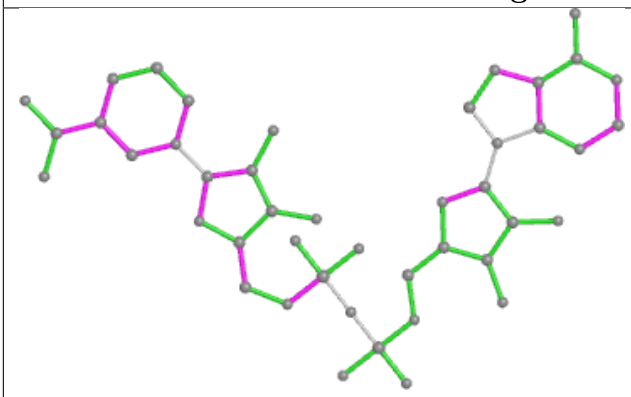


Torsions

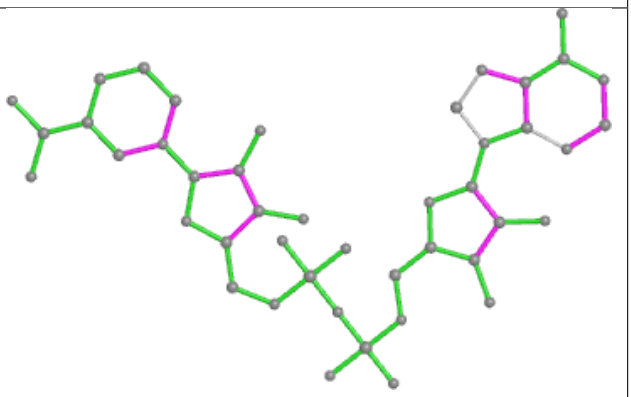


Rings

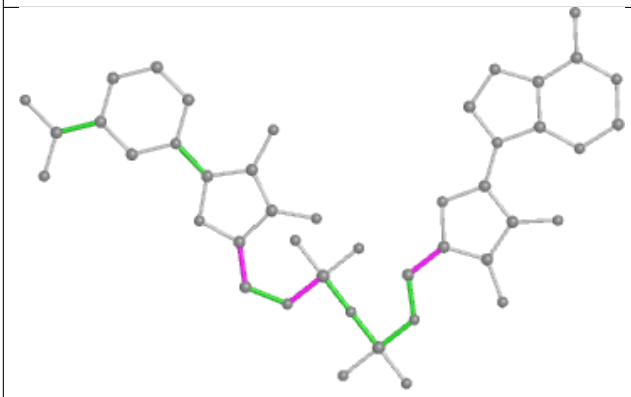
Ligand NAD D 3601



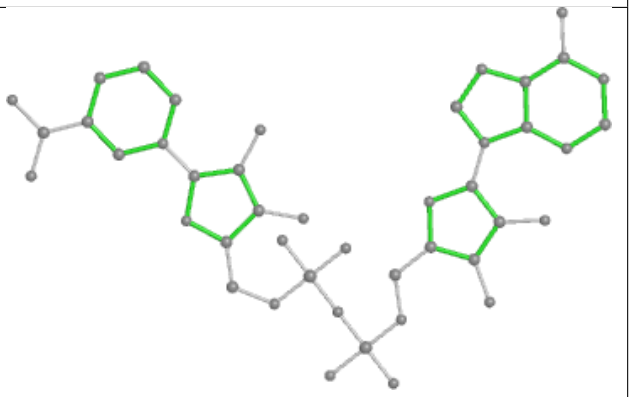
Bond lengths



Bond angles

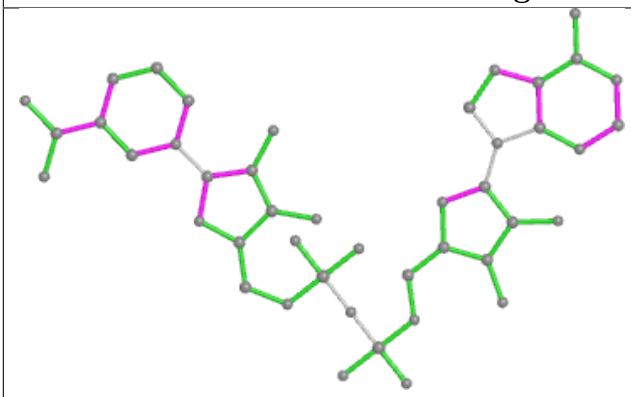


Torsions

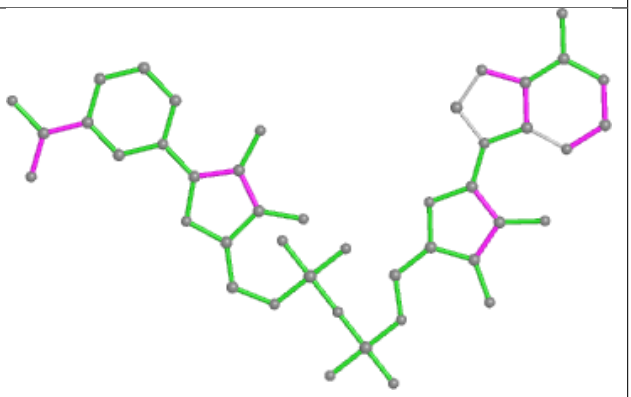


Rings

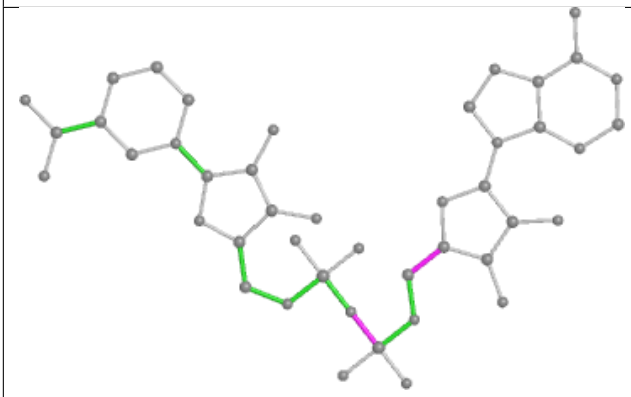
Ligand NAD F 5601



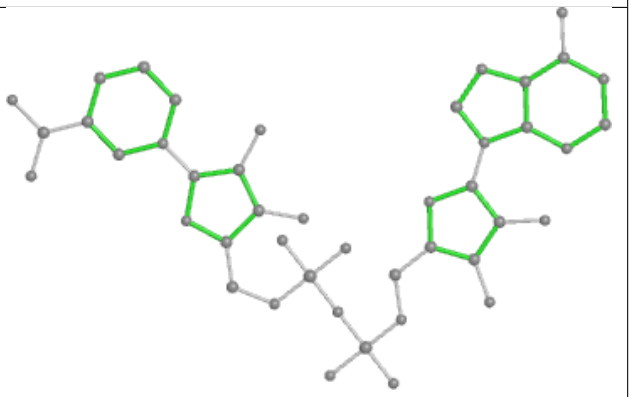
Bond lengths



Bond angles

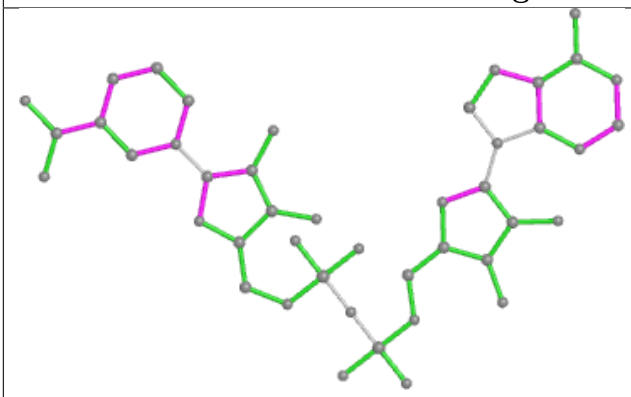


Torsions

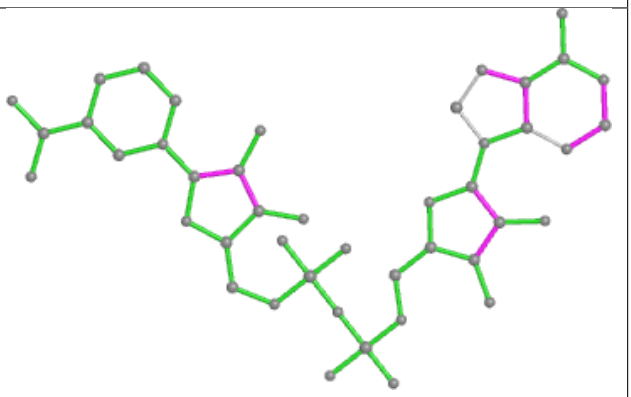


Rings

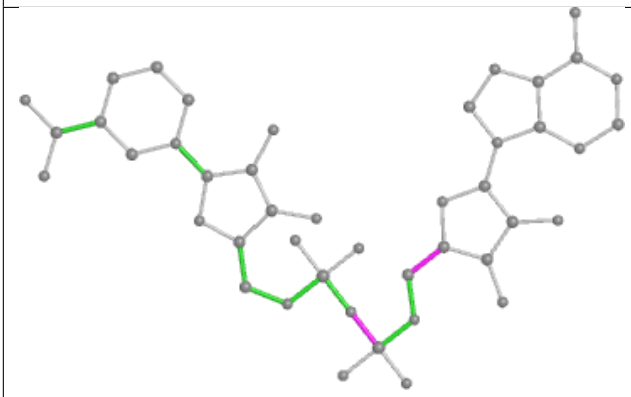
Ligand NAD E 4601



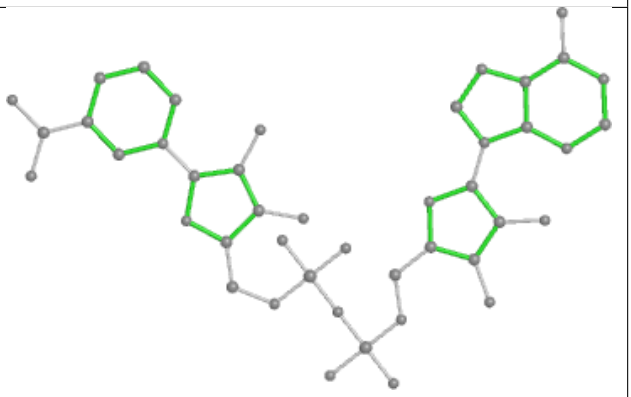
Bond lengths



Bond angles

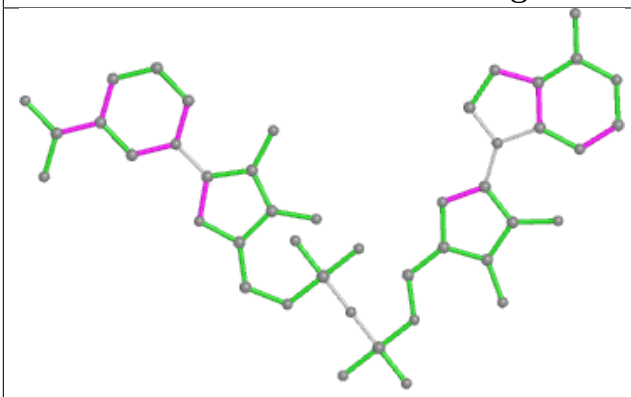


Torsions

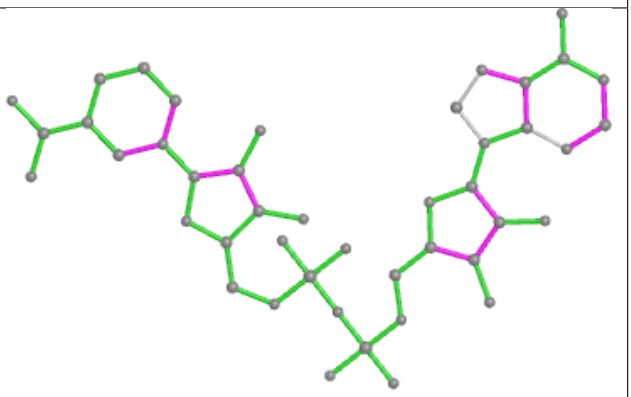


Rings

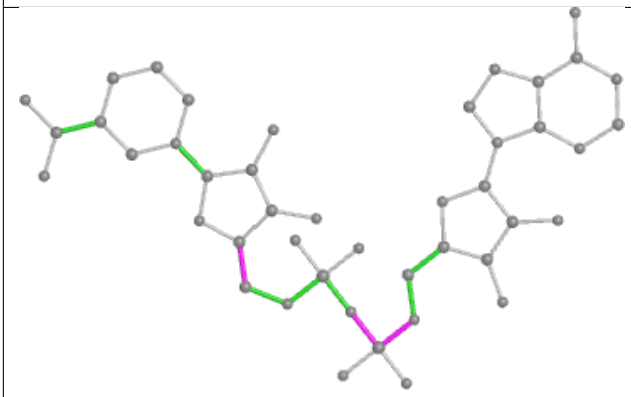
Ligand NAD H 7602



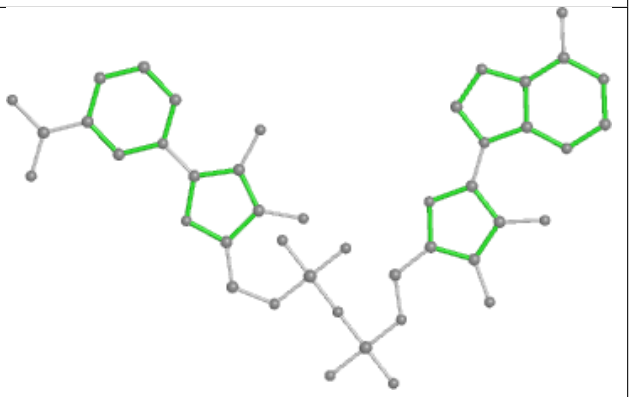
Bond lengths



Bond angles

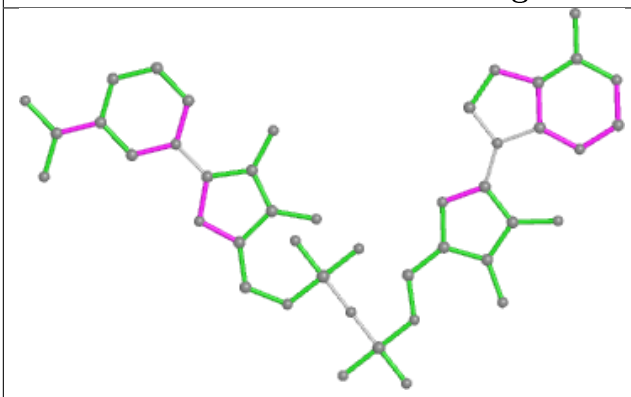


Torsions

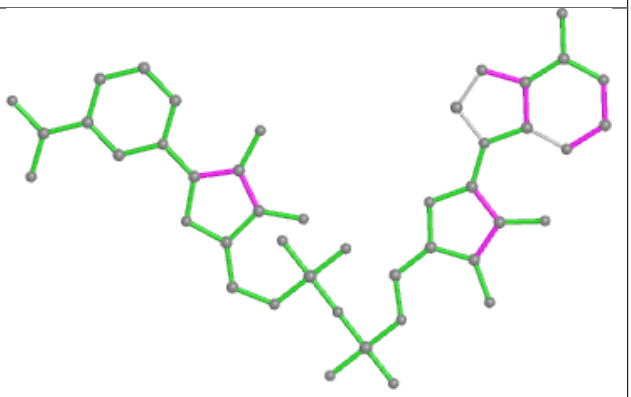


Rings

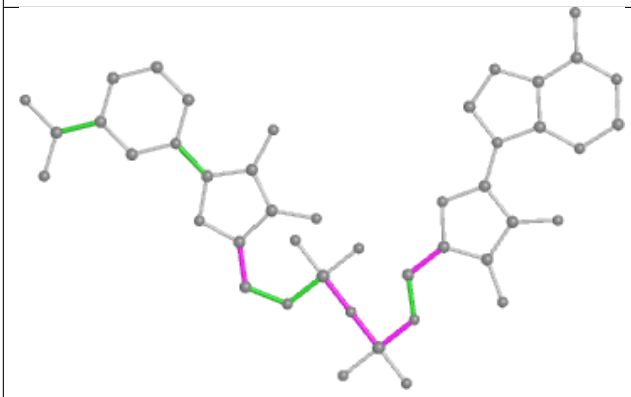
Ligand NAD B 1601



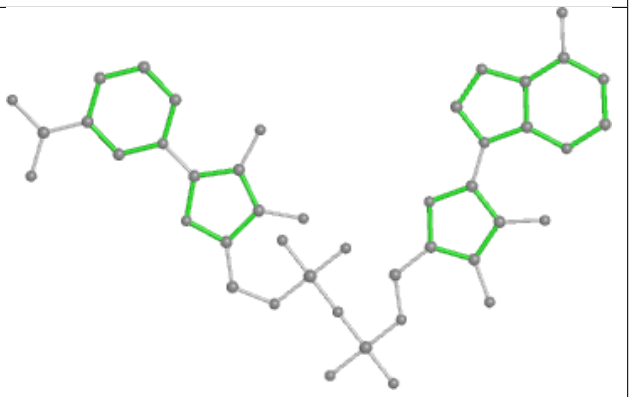
Bond lengths



Bond angles

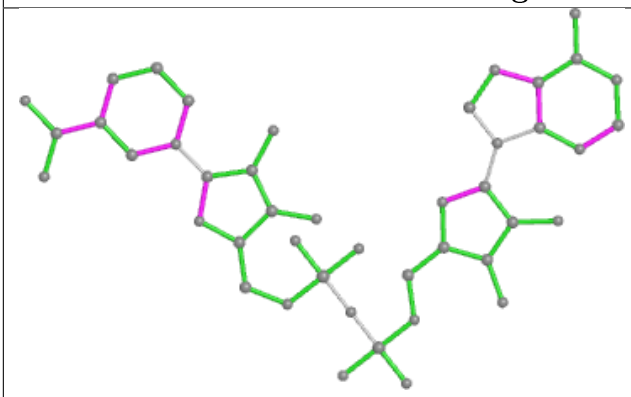


Torsions

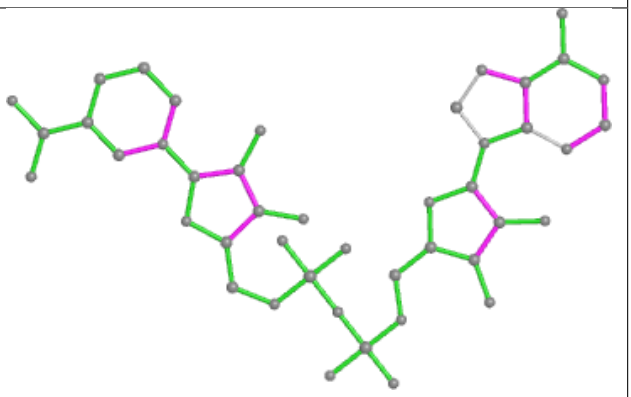


Rings

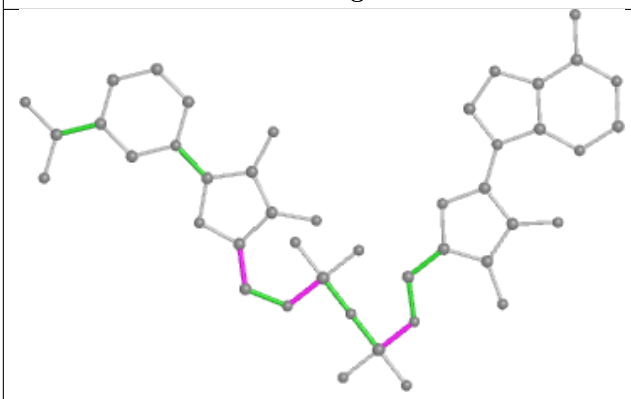
Ligand NAD C 2602



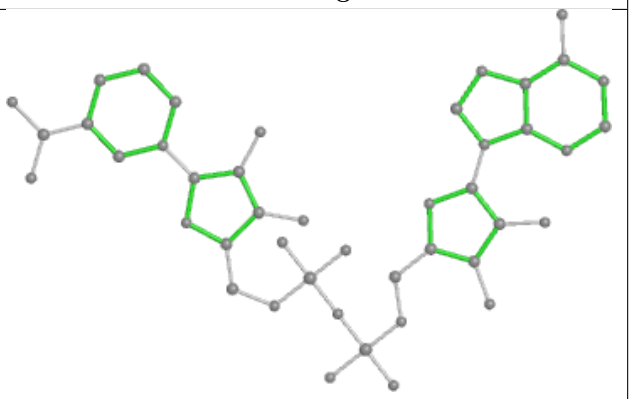
Bond lengths



Bond angles

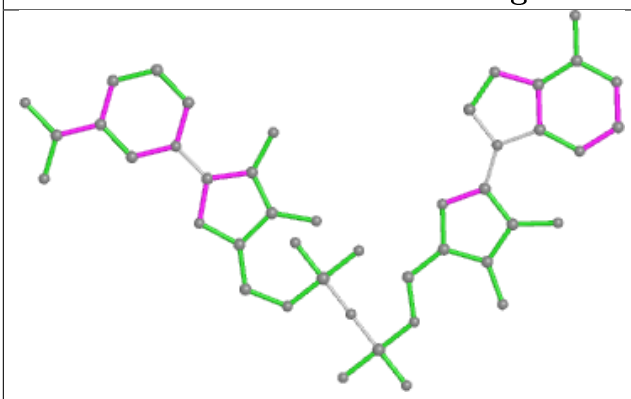


Torsions

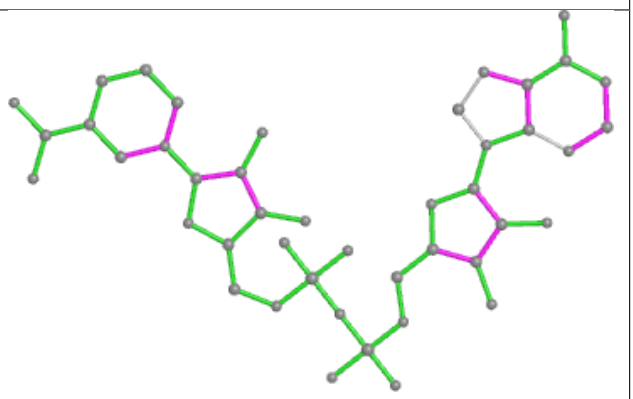


Rings

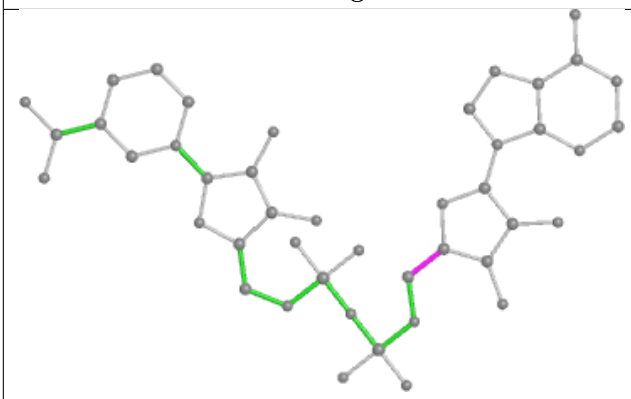
Ligand NAD G 6601



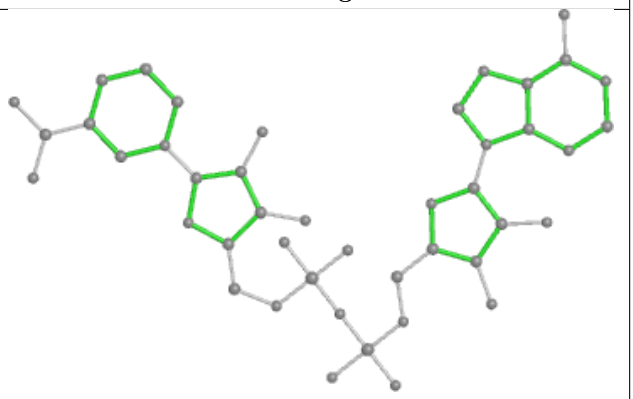
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.