



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:01 PM GMT

PDB ID : 1MX9  
Title : Crystal Structure of Human Liver Carboxylesterase in complexed with naloxone methiodide, a heroin analogue  
Authors : Bencharit, S.; Morton, C.L.; Xue, Y.; Potter, P.M.; Redinbo, M.R.  
Deposited on : 2002-10-01  
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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

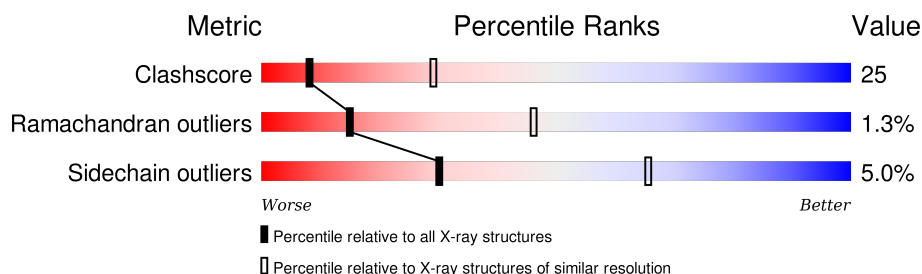
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	548	
1	B	548	
1	C	548	
1	D	548	
1	E	548	
1	F	548	
1	G	548	

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Mol	Chain	Length	Quality of chain
1	H	548	
1	I	548	
1	J	548	
1	K	548	
1	L	548	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	J	479	-	-	X	-
3	NLX	A	1	X	-	X	-
3	NLX	B	2	X	-	X	-
3	NLX	C	3	X	-	X	-
3	NLX	D	4	X	-	X	-
3	NLX	E	5	X	-	X	-
3	NLX	F	6	X	-	X	-
3	NLX	G	1	X	-	X	-
3	NLX	H	2	X	-	X	-
3	NLX	I	3	X	-	X	-
3	NLX	J	4	X	-	X	-
3	NLX	K	5	X	-	X	-
3	NLX	L	6	X	-	X	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 51134 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 liver Carboxylesterase I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	532	Total	C	N	O	S	0	0	0
			4130	2662	685	763	20			
1	B	532	Total	C	N	O	S	0	0	0
			4130	2662	685	763	20			
1	C	531	Total	C	N	O	S	0	0	0
			4124	2659	684	761	20			
1	D	533	Total	C	N	O	S	0	0	0
			4135	2665	686	764	20			
1	E	531	Total	C	N	O	S	0	0	0
			4124	2659	684	761	20			
1	F	531	Total	C	N	O	S	0	0	0
			4124	2659	684	761	20			
1	G	532	Total	C	N	O	S	0	0	0
			4130	2662	685	763	20			
1	H	531	Total	C	N	O	S	0	0	0
			4124	2659	684	761	20			
1	I	531	Total	C	N	O	S	0	0	0
			4124	2659	684	761	20			
1	J	532	Total	C	N	O	S	0	0	0
			4130	2662	685	763	20			
1	K	531	Total	C	N	O	S	0	0	0
			4124	2659	684	761	20			
1	L	531	Total	C	N	O	S	0	0	0
			4124	2659	684	761	20			

There are 12 discrepancies between the modelled and reference sequences:

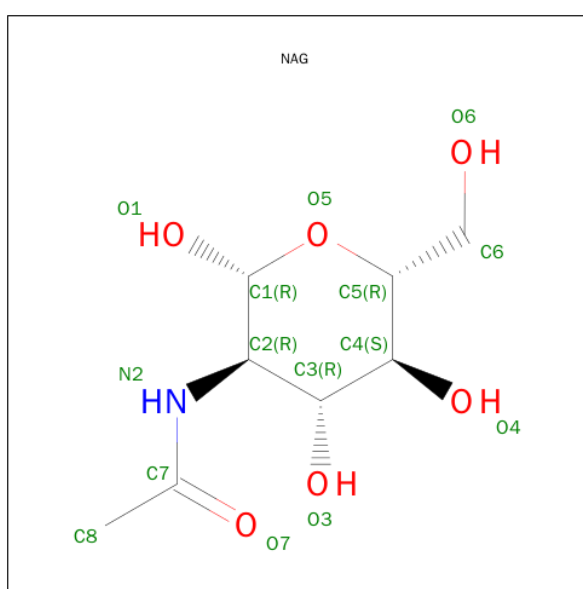
Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	GLN	DELETION	UNP P23141
B	?	-	GLN	DELETION	UNP P23141
C	?	-	GLN	DELETION	UNP P23141
D	?	-	GLN	DELETION	UNP P23141
E	?	-	GLN	DELETION	UNP P23141

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Chain	Residue	Modelled	Actual	Comment	Reference
F	?	-	GLN	DELETION	UNP P23141
G	?	-	GLN	DELETION	UNP P23141
H	?	-	GLN	DELETION	UNP P23141
I	?	-	GLN	DELETION	UNP P23141
J	?	-	GLN	DELETION	UNP P23141
K	?	-	GLN	DELETION	UNP P23141
L	?	-	GLN	DELETION	UNP P23141

- Molecule 2 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



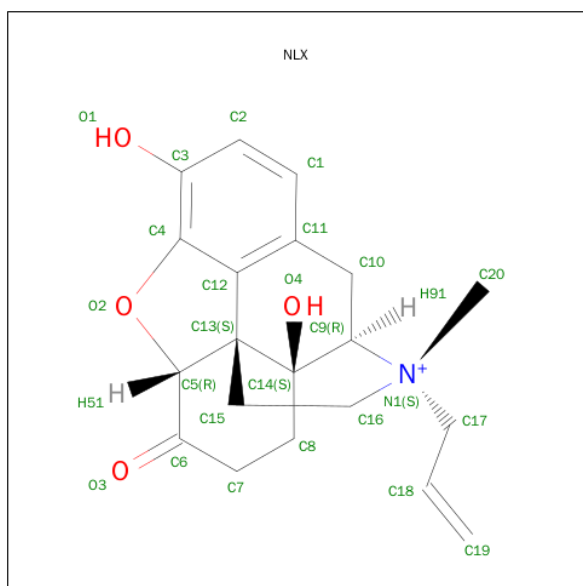
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	E	1	Total	C	N	O	0	0
			14	8	1	5		
2	F	1	Total	C	N	O	0	0
			14	8	1	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	G	1	Total	C	N	O	0	0
			14	8	1	5		
2	H	1	Total	C	N	O	0	0
			14	8	1	5		
2	I	1	Total	C	N	O	0	0
			14	8	1	5		
2	J	1	Total	C	N	O	0	0
			14	8	1	5		
2	K	1	Total	C	N	O	0	0
			14	8	1	5		
2	L	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is (5A,17R)-4,5-EPOXY-3,14-DIHYDROXY-17-METHYL-6-OXO-17-(2-PROPENYL)-MORPHINANIUM (three-letter code: NLX) (formula: C<sub>20</sub>H<sub>24</sub>NO<sub>4</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			25	20	1	4		
3	B	1	Total	C	N	O	0	0
			25	20	1	4		
3	C	1	Total	C	N	O	0	0
			25	20	1	4		
3	D	1	Total	C	N	O	0	0
			25	20	1	4		
3	E	1	Total	C	N	O	0	0
			25	20	1	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	F	1	Total	C	N	O	0	0
			25	20	1	4		
3	G	1	Total	C	N	O	0	0
			25	20	1	4		
3	H	1	Total	C	N	O	0	0
			25	20	1	4		
3	I	1	Total	C	N	O	0	0
			25	20	1	4		
3	J	1	Total	C	N	O	0	0
			25	20	1	4		
3	K	1	Total	C	N	O	0	0
			25	20	1	4		
3	L	1	Total	C	N	O	0	0
			25	20	1	4		

- Molecule 4 is water.

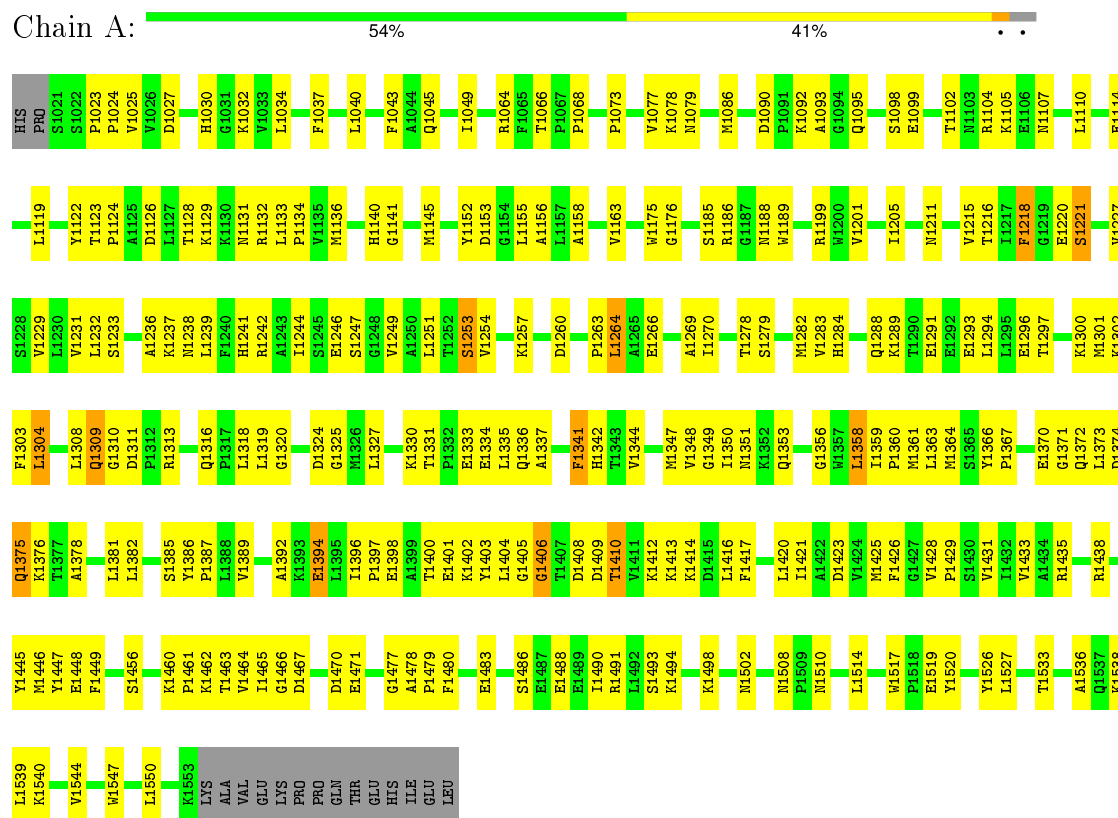
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	87	Total	O	0	0
			87	87		
4	B	120	Total	O	0	0
			120	120		
4	C	98	Total	O	0	0
			98	98		
4	D	119	Total	O	0	0
			119	119		
4	E	112	Total	O	0	0
			112	112		
4	F	91	Total	O	0	0
			91	91		
4	G	69	Total	O	0	0
			69	69		
4	H	95	Total	O	0	0
			95	95		
4	I	80	Total	O	0	0
			80	80		
4	J	110	Total	O	0	0
			110	110		
4	K	73	Total	O	0	0
			73	73		
4	L	75	Total	O	0	0
			75	75		

### 3 Residue-property plots

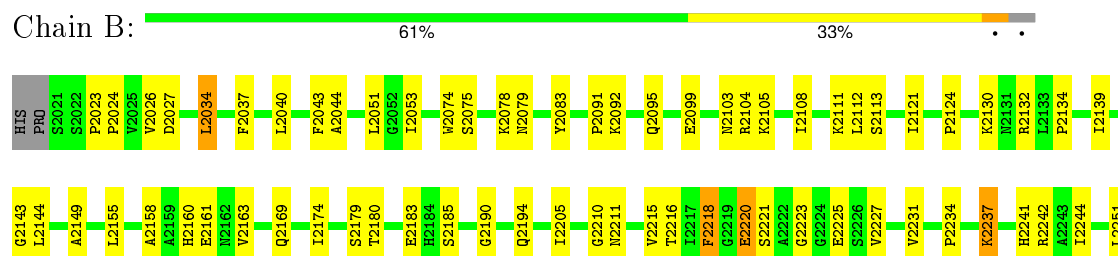
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

Note EDS was not executed.

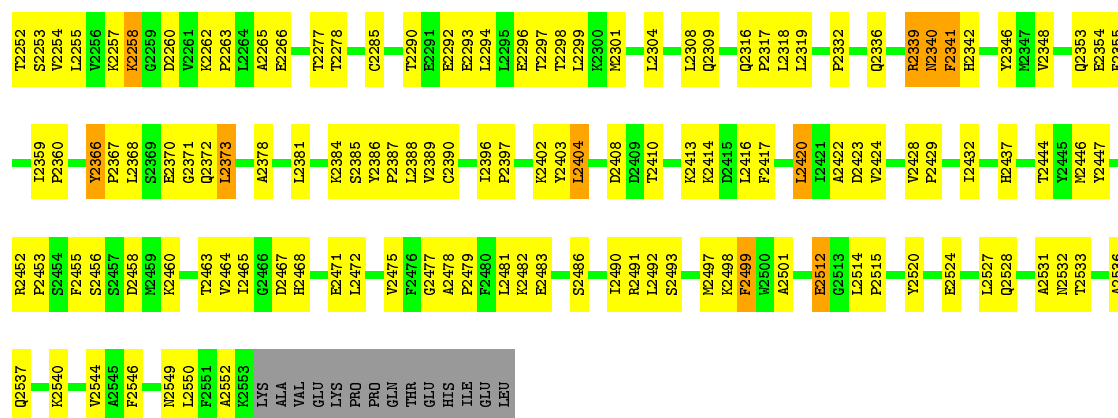
- Molecule 1: liver Carboxylesterase I



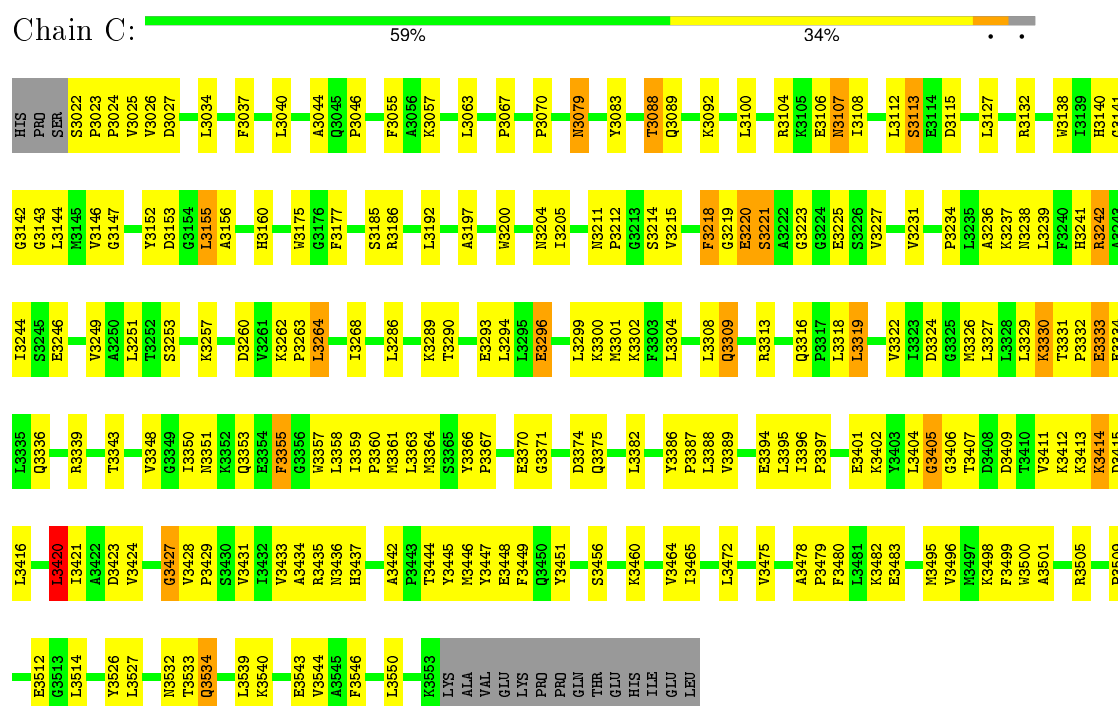
- Molecule 1: liver Carboxylesterase I



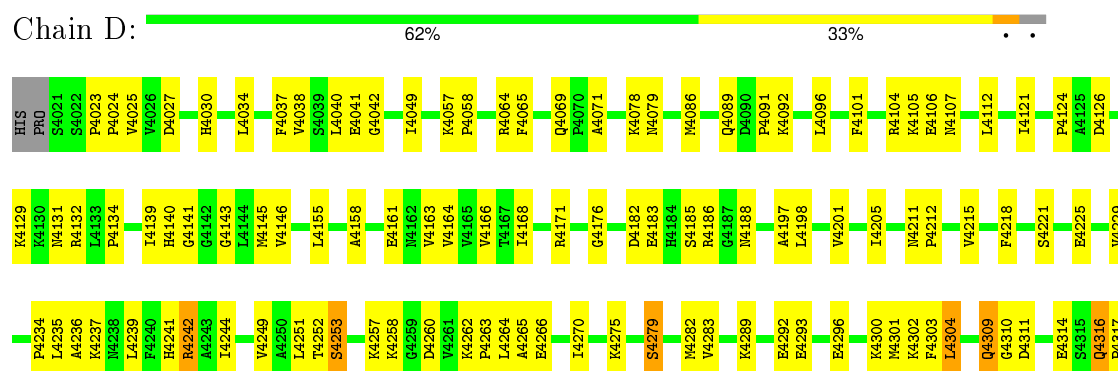


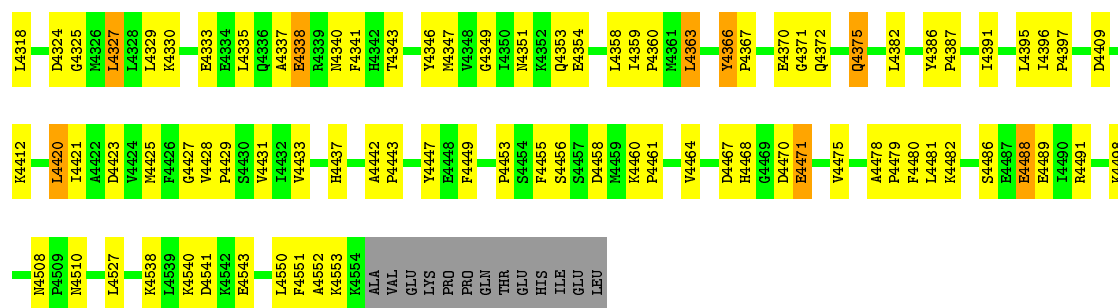


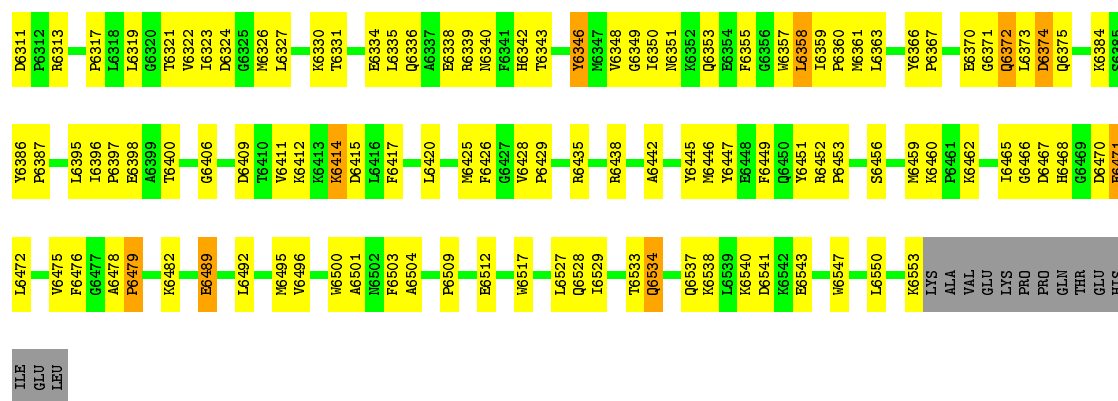
- Molecule 1: liver Carboxylesterase I



- Molecule 1: liver Carboxylesterase I

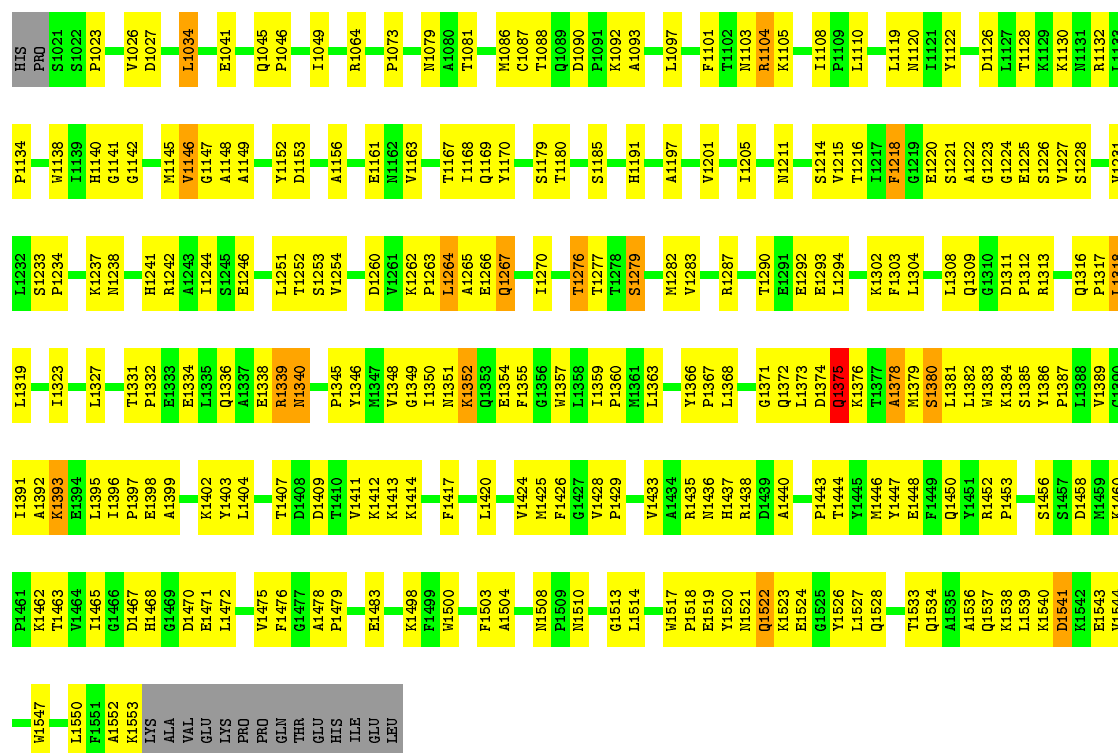






• Molecule 1: liver Carboxylesterase I

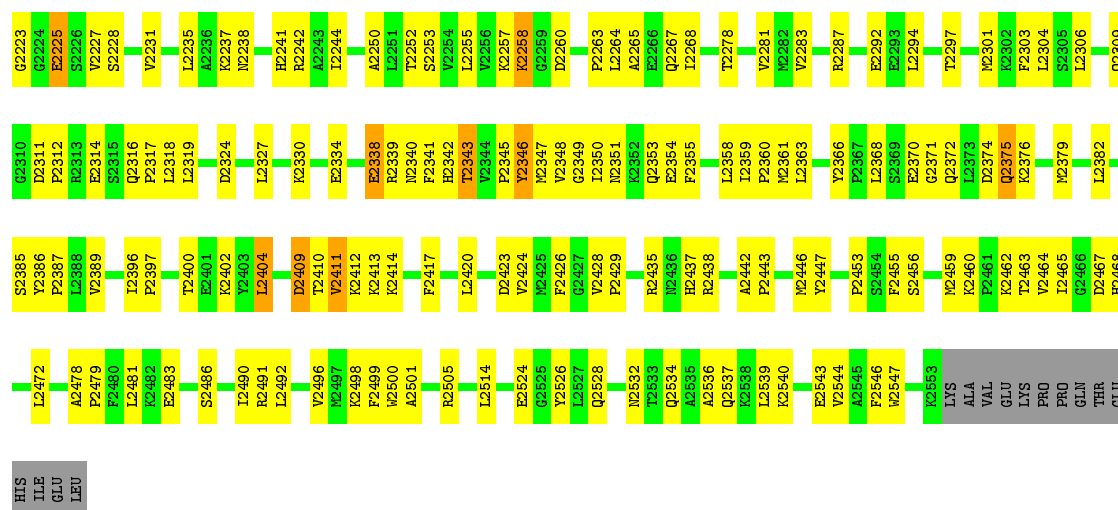
Chain G: 53% 41%



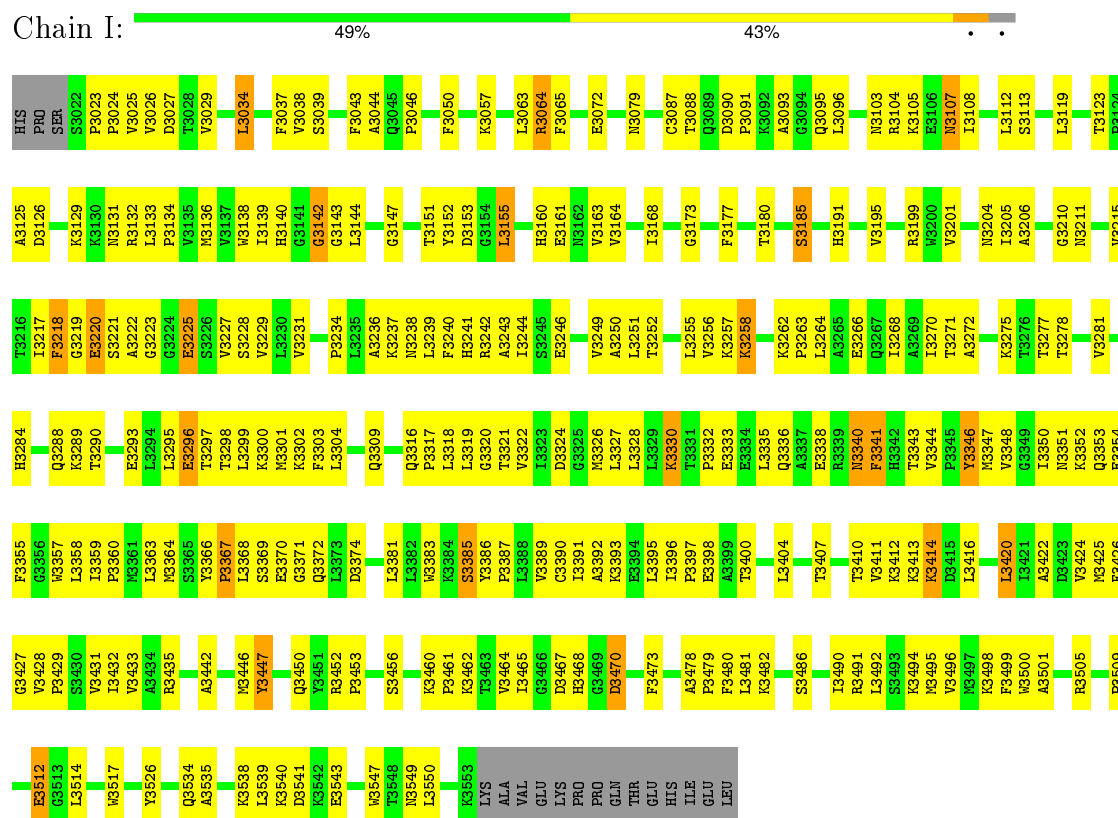
• Molecule 1: liver Carboxylesterase I

Chain H: 57% 38%

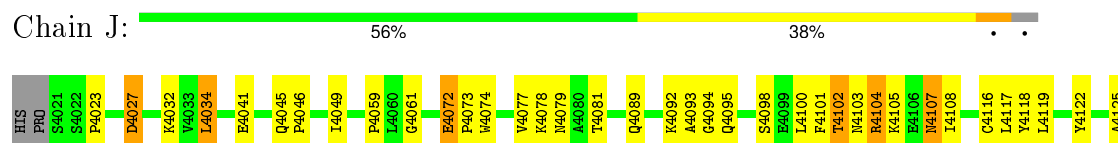


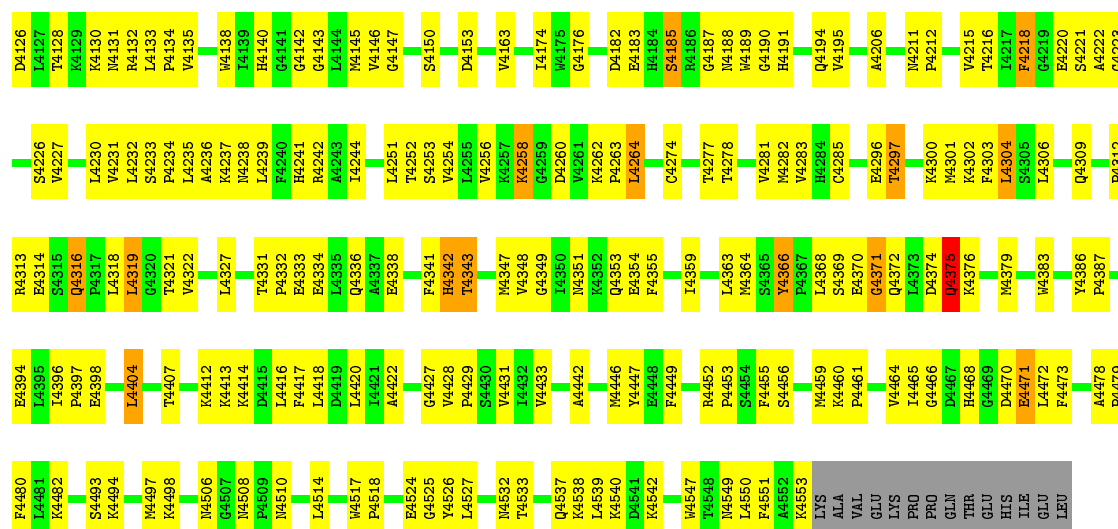


### • Molecule 1: liver Carboxylesterase I

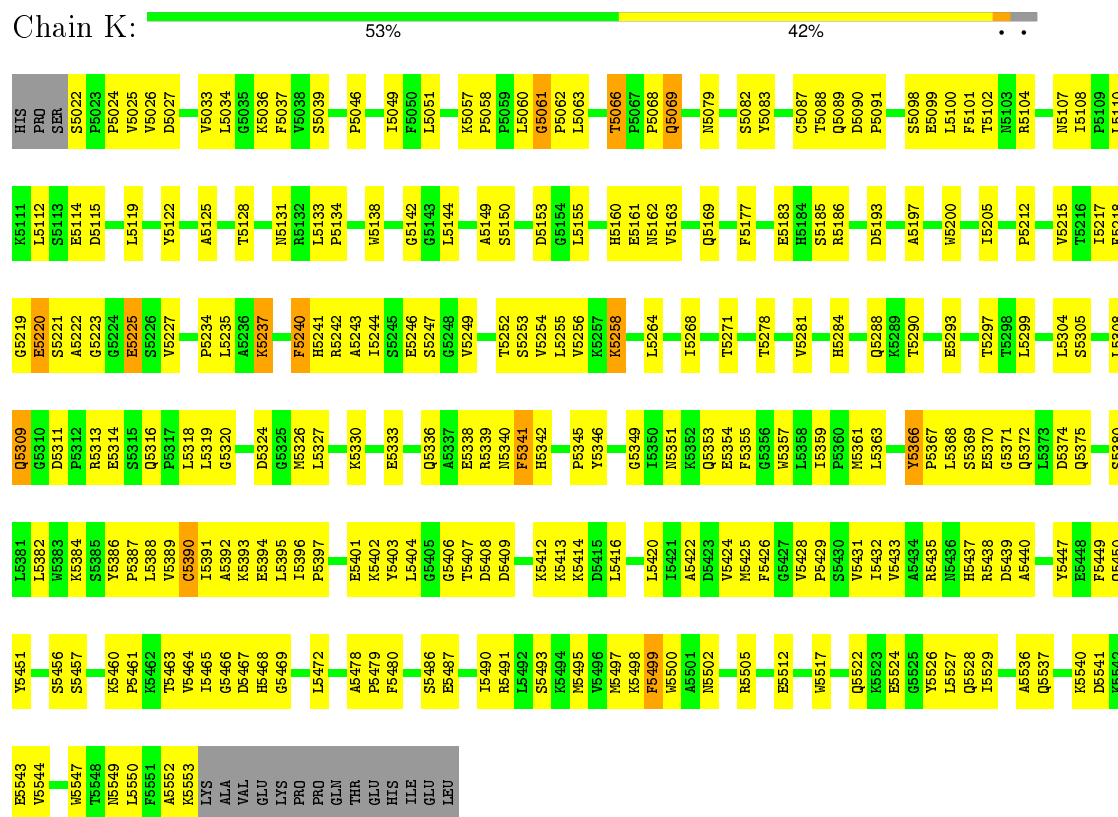


### • Molecule 1: liver Carboxylesterase I

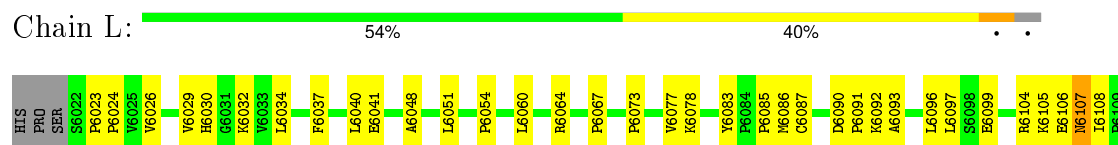




- Molecule 1: liver Carboxylesterase I



- Molecule 1: liver Carboxylesterase I



M6547	I6465	L6373	V6283	L6198	I6110
T6546	H6468	D6374	I6286	M6204	K6111
M6549		Q6375		I6205	L6112
L6550	E6471	A6378	K6289	A6206	S6113
	L6472		T6290	S6207	E6114
		L6382	E6291		D6115
	V6475	M6383	E6292	V6215	
			E6293	T6216	I6121
	A6478	Y6386	T6297	I6217	Y6122
	P6479	P6387		F6218	T6123
	F6480			G6219	P6124
	L6481	K6393	K6302	E6220	A6125
		E6394	F6303	S6221	D6126
	G6484	I6395	I6304	A6222	L6127
	A6485	I6396		G6223	T6128
	S6486		D6311	G6224	K6129
	E6487	T6400	P6312	G6225	K6130
		E6401	R6313	S6226	
				V6227	L6133
	L6492	D6409	Q6316		P6134
	S6493	T6410	P6317	S6233	V6135
		V6496	L6318	P6234	M6136
	V6496	M6497	L6319	L6235	V6137
	K6498	K6413		A6236	M6138
	F6499	K6414	V6322	K6237	I6139
	M6500	D6415	I6323	M6238	H6140
	A6501	L6416	D6324		G6141
		F6417	G6325	H6241	G6142
	A6504	L6418	M6326	R6242	G6143
		D6419	L6327		L6144
	P6509	L6420		I6244	M6145
			E6333	S6245	
	M6517	F6426		E6246	A6149
		G6427	Q6336		L6155
	Y6520	V6428		L6251	A6156
		P6429	R6339	T6252	
	K6523			S6253	E6161
	E6524	I6432	H6342	V6254	R6162
	G6525	V6433		L6255	V6163
	Y6526	A6434	M6347	V6256	
	L6527	R6435	V6348	K6257	Q6169
	Q6528		G6349	K6258	Y6170
	I6529	D6439	I6350	G6259	R6171
	G6530		M6351	D6260	
	A6531	T6444		V6261	I6174
	M6532	Y6445	F6355	K6262	M6175
	T6533	M6446	G6356	P6263	G6176
	Q6534	Y6447	M6357	L6264	F6177
	A6535		L6358	A6265	
	A6536	R6452	I6359	E6266	D6182
	Q6537	P6453	P6360	Q6267	E6183
	K6538		M6361	I6268	H6184
	L6539	S6456	L6363		S6185
	K6540			T6271	R6186
	D6541	M6459	Y6366		G6187
		K6460	P6367	T6278	M6188
	V6544			S6279	
	A6545	T6463	G6371	A6280	Q6194
	F6546	V6464	Q6372		

K6553
LYS
ALA
VAL
GLU
LYS
LYS
PRO
PRO
GLN
THR
GLU
HIS
ILE
GLU
LEU

## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	91.17Å 120.71Å 177.02Å 90.28° 89.32° 99.22°	Depositor
Resolution (Å)	29.82 – 2.90	Depositor
% Data completeness (in resolution range)	95.7 (29.82-2.90)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.214 , 0.280	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	51134	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.38	0/4236	0.62	0/5754
1	B	0.41	0/4236	0.66	2/5754 (0.0%)
1	C	0.42	0/4230	0.65	2/5746 (0.0%)
1	D	0.41	0/4241	0.63	0/5761
1	E	0.40	0/4230	0.64	1/5746 (0.0%)
1	F	0.38	0/4230	0.62	0/5746
1	G	0.36	0/4236	0.60	0/5754
1	H	0.39	0/4230	0.63	0/5746
1	I	0.36	0/4230	0.61	0/5746
1	J	0.39	0/4236	0.62	0/5754
1	K	0.36	0/4230	0.60	0/5746
1	L	0.37	0/4230	0.63	1/5746 (0.0%)
All	All	0.39	0/50795	0.63	6/68999 (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	E	0	1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	3420	LEU	CA-CB-CG	5.80	128.63	115.30
1	C	3388	LEU	CB-CG-CD2	-5.50	101.66	111.00
1	B	2339	ARG	N-CA-C	5.37	125.50	111.00
1	B	2075	SER	N-CA-C	5.33	125.41	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	6140	HIS	N-CA-C	5.01	124.53	111.00
1	E	5075	SER	N-CA-C	5.00	124.50	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	5118	TYR	Sidechain

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4130	0	4132	231	0
1	B	4130	0	4132	182	0
1	C	4124	0	4127	180	0
1	D	4135	0	4134	165	0
1	E	4124	0	4127	200	0
1	F	4124	0	4127	192	0
1	G	4130	0	4132	237	0
1	H	4124	0	4127	194	0
1	I	4124	0	4127	232	0
1	J	4130	0	4134	216	0
1	K	4124	0	4127	226	0
1	L	4124	0	4127	244	0
2	A	28	0	26	3	0
2	B	14	0	13	4	0
2	C	14	0	13	0	0
2	D	14	0	13	4	0
2	E	14	0	13	2	0
2	F	14	0	13	0	0
2	G	14	0	13	4	0
2	H	14	0	13	1	0
2	I	14	0	13	1	0
2	J	14	0	13	7	0
2	K	14	0	13	1	0
2	L	14	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	25	0	23	20	0
3	B	25	0	23	21	0
3	C	25	0	19	27	0
3	D	25	0	24	15	0
3	E	25	0	24	18	0
3	F	25	0	21	23	0
3	G	25	0	23	12	0
3	H	25	0	23	30	0
3	I	25	0	24	19	0
3	J	25	0	24	20	0
3	K	25	0	24	18	0
3	L	25	0	24	23	0
4	A	87	0	0	9	0
4	B	120	0	0	12	0
4	C	98	0	0	10	0
4	D	119	0	0	9	0
4	E	112	0	0	16	0
4	F	91	0	0	8	0
4	G	69	0	0	10	0
4	H	95	0	0	10	0
4	I	80	0	0	10	0
4	J	110	0	0	8	0
4	K	73	0	0	11	0
4	L	75	0	0	15	0
All	All	51134	0	49998	2453	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 25.

All (2453) 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)
3:C:3:NLX:N1	3:C:3:NLX:C9	1.69	1.56
3:C:3:NLX:C9	3:C:3:NLX:C14	1.78	1.55
1:D:4343:THR:HB	1:D:4442:ALA:HB2	1.17	1.13
1:H:2304:LEU:HB3	3:H:2:NLX:H201	1.28	1.11
1:C:3364:MET:CE	3:C:3:NLX:H181	1.83	1.08
1:A:1251:LEU:HD11	1:A:1336:GLN:HE22	1.18	1.08
1:D:4359:ILE:HG23	3:D:4:NLX:H82	1.39	1.04
1:H:2363:LEU:HB3	3:H:2:NLX:H181	1.36	1.03
1:F:6097:LEU:HD22	3:F:6:NLX:H192	1.39	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4363:LEU:HB3	3:D:4:NLX:H181	1.43	1.01
1:G:1134:PRO:HG2	1:G:1163:VAL:HG12	1.44	1.00
1:B:2373:LEU:HD21	1:B:2378:ALA:HB2	1.43	0.99
1:A:1498:LYS:HD2	1:A:1514:LEU:HD11	1.45	0.98
1:K:5258:LYS:H	1:K:5258:LYS:HD2	1.26	0.97
1:A:1025:VAL:HG22	1:A:1034:LEU:HD23	1.45	0.97
1:B:2234:PRO:HA	1:B:2237:LYS:HE2	1.48	0.96
3:C:3:NLX:C9	3:C:3:NLX:C16	2.44	0.95
1:C:3215:VAL:H	1:C:3241:HIS:HD2	1.00	0.95
1:C:3242:ARG:HH11	1:C:3242:ARG:HG2	1.29	0.94
1:J:4216:THR:HG23	1:J:4242:ARG:HB2	1.50	0.94
1:G:1215:VAL:H	1:G:1241:HIS:HD2	1.14	0.94
1:C:3364:MET:HE1	3:C:3:NLX:H181	1.47	0.93
1:B:2359:ILE:HG12	3:B:2:NLX:H71	1.51	0.92
1:K:5237:LYS:HA	1:K:5237:LYS:HE2	1.49	0.92
1:I:3490:ILE:HG22	1:I:3494:LYS:HD2	1.49	0.92
1:E:5363:LEU:CB	3:E:5:NLX:H201	1.99	0.92
1:H:2359:ILE:HG23	3:H:2:NLX:H82	1.49	0.92
1:J:4363:LEU:HD13	3:J:4:NLX:H181	1.52	0.92
1:E:5304:LEU:HD13	3:E:5:NLX:H181	1.52	0.92
1:G:1079:ASN:HB2	2:G:179:NAG:H82	1.50	0.91
1:D:4215:VAL:H	1:D:4241:HIS:HD2	1.14	0.91
1:B:2091:PRO:HG3	1:B:2112:LEU:HD11	1.51	0.91
1:A:1414:LYS:HZ2	1:F:6370:GLU:HA	1.36	0.91
1:I:3290:THR:OG1	1:I:3293:GLU:HG3	1.71	0.90
1:D:4134:PRO:HG2	1:D:4163:VAL:HG12	1.52	0.90
1:L:6363:LEU:HD13	3:L:6:NLX:H203	1.54	0.90
1:L:6134:PRO:HG2	1:L:6163:VAL:HG12	1.53	0.90
1:L:6215:VAL:H	1:L:6241:HIS:HD2	1.18	0.89
1:E:5363:LEU:HB3	3:E:5:NLX:H201	1.51	0.89
1:H:2404:LEU:HB3	1:H:2413:LYS:HG3	1.53	0.89
1:C:3143:GLY:HA3	3:C:3:NLX:H152	1.52	0.89
1:A:1134:PRO:HG2	1:A:1163:VAL:HG12	1.53	0.89
1:G:1302:LYS:HG3	1:L:6092:LYS:NZ	1.88	0.88
1:A:1215:VAL:H	1:A:1241:HIS:HD2	1.14	0.88
1:E:5404:LEU:HB3	1:E:5413:LYS:HG2	1.54	0.88
1:B:2359:ILE:HG23	3:B:2:NLX:H82	1.56	0.87
1:G:1302:LYS:HG3	1:L:6092:LYS:HZ3	1.38	0.87
1:B:2134:PRO:HG2	1:B:2163:VAL:HG12	1.57	0.86
1:H:2304:LEU:CB	3:H:2:NLX:H201	2.05	0.86
1:G:1396:ILE:HB	1:G:1397:PRO:HD3	1.56	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:5091:PRO:HG3	1:E:5112:LEU:HD11	1.57	0.86
1:K:5234:PRO:HA	1:K:5237:LYS:HE3	1.57	0.85
1:C:3215:VAL:H	1:C:3241:HIS:CD2	1.91	0.85
1:G:1404:LEU:HD13	1:G:1413:LYS:HG2	1.58	0.85
1:E:5304:LEU:HD22	3:E:5:N LX:H102	1.59	0.85
1:H:2134:PRO:HG2	1:H:2163:VAL:HG12	1.57	0.85
1:L:6235:LEU:HD12	1:L:6327:LEU:HD12	1.58	0.85
1:K:5371:GLY:HA2	1:K:5414:LYS:HD3	1.57	0.85
1:F:6134:PRO:HG2	1:F:6163:VAL:HG12	1.59	0.84
1:K:5304:LEU:HD13	3:K:5:N LX:H181	1.59	0.84
1:B:2318:LEU:HG	3:B:2:N LX:H171	1.58	0.84
1:K:5221:SER:OG	3:K:5:N LX:H71	1.78	0.84
1:E:5490:ILE:O	1:E:5494:LYS:HG3	1.76	0.84
1:K:5221:SER:OG	1:K:5222:ALA:N	2.09	0.84
1:D:4292:GLU:O	1:D:4296:GLU:HG3	1.78	0.83
1:G:1304:LEU:HG	3:G:1:N LX:H203	1.60	0.83
1:D:4304:LEU:CG	3:D:4:N LX:H201	2.08	0.83
1:L:6215:VAL:H	1:L:6241:HIS:CD2	1.96	0.83
1:C:3257:LYS:HD3	4:C:7152:HOH:O	1.78	0.82
1:J:4468:HIS:NE2	3:J:4:N LX:H21	1.94	0.82
1:A:1414:LYS:NZ	1:F:6370:GLU:HA	1.93	0.82
1:I:3370:GLU:HG3	1:J:4461:PRO:HG3	1.59	0.82
1:H:2263:PRO:O	1:H:2267:GLN:HG3	1.79	0.82
1:F:6034:LEU:HD12	1:F:6079:ASN:ND2	1.93	0.82
1:A:1353:GLN:NE2	1:A:1465:ILE:H	1.77	0.82
1:L:6023:PRO:HB2	1:L:6034:LEU:HD21	1.61	0.82
1:A:1461:PRO:HG2	1:A:1464:VAL:HG23	1.62	0.82
1:D:4242:ARG:HG2	1:D:4242:ARG:HH11	1.44	0.82
1:D:4304:LEU:CB	3:D:4:N LX:H201	2.10	0.82
1:C:3318:LEU:HD11	3:C:3:N LX:H151	1.60	0.81
1:H:2363:LEU:HD13	3:H:2:N LX:H101	1.62	0.81
1:H:2221:SER:HB3	3:H:2:N LX:O1	1.81	0.81
1:L:6105:LYS:HD3	1:L:6106:GLU:HG3	1.60	0.81
1:A:1331:THR:OG1	1:A:1334:GLU:HG2	1.79	0.81
1:C:3088:THR:HA	1:C:3112:LEU:HD22	1.62	0.81
1:E:5304:LEU:HD21	1:E:5318:LEU:HD21	1.62	0.81
1:K:5115:ASP:OD2	1:L:6280:ALA:HB3	1.81	0.81
1:F:6254:VAL:HG21	3:F:6:N LX:O1	1.80	0.81
1:C:3343:THR:HB	1:C:3442:ALA:HB2	1.62	0.80
1:F:6363:LEU:HD13	3:F:6:N LX:H171	1.62	0.80
1:K:5363:LEU:CB	3:K:5:N LX:H201	2.12	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3364:MET:SD	3:C:3:NLX:H181	2.22	0.80
1:A:1304:LEU:HB3	3:A:1:NLX:H203	1.63	0.80
1:K:5083:TYR:CE2	1:K:5108:ILE:HD13	2.16	0.79
1:G:1382:LEU:HD22	1:G:1420:LEU:HD21	1.62	0.79
1:F:6331:THR:OG1	1:F:6334:GLU:HG3	1.81	0.79
1:A:1375:GLN:HE22	1:A:1400:THR:HG22	1.47	0.79
1:A:1092:LYS:HE3	4:A:8088:HOH:O	1.83	0.79
1:F:6215:VAL:H	1:F:6241:HIS:HD2	1.28	0.79
1:K:5235:LEU:HD12	1:K:5327:LEU:HD12	1.65	0.79
1:K:5215:VAL:H	1:K:5241:HIS:HD2	1.28	0.79
1:E:5407:THR:HG21	1:E:5412:LYS:HB2	1.65	0.79
1:A:1363:LEU:HD13	3:A:1:NLX:H101	1.63	0.78
1:I:3371:GLY:O	1:I:3411:VAL:HA	1.82	0.78
1:L:6258:LYS:H	1:L:6258:LYS:HD3	1.45	0.78
1:A:1376:LYS:HD3	1:F:6462:LYS:HE2	1.62	0.78
1:I:3318:LEU:HG	3:I:3:NLX:C19	2.12	0.78
1:B:2079:ASN:HD22	2:B:279:NAG:H82	1.49	0.78
1:K:5134:PRO:HG2	1:K:5163:VAL:HG12	1.62	0.78
1:B:2079:ASN:ND2	2:B:279:NAG:H82	1.99	0.78
1:B:2317:PRO:HB2	3:B:2:NLX:H192	1.64	0.78
1:J:4428:VAL:HB	1:J:4429:PRO:HD3	1.64	0.78
1:F:6216:THR:HG23	1:F:6242:ARG:HB2	1.66	0.78
1:G:1104:ARG:NH1	1:G:1153:ASP:HB2	1.99	0.77
1:J:4338:GLU:HG3	1:J:4338:GLU:O	1.83	0.77
1:F:6290:THR:HG23	1:F:6293:GLU:OE1	1.85	0.77
1:L:6304:LEU:HD22	3:L:6:NLX:H172	1.64	0.77
1:A:1363:LEU:HD22	3:A:1:NLX:H181	1.64	0.77
1:L:6114:GLU:OE1	1:L:6291:GLU:HB2	1.84	0.77
1:J:4215:VAL:H	1:J:4241:HIS:HD2	1.33	0.77
1:J:4132:ARG:HH12	1:J:4206:ALA:CB	1.98	0.77
1:I:3234:PRO:O	1:I:3237:LYS:HG2	1.85	0.77
1:B:2220:GLU:OE1	1:B:2221:SER:HB2	1.84	0.77
1:B:2359:ILE:HG12	3:B:2:NLX:C7	2.14	0.77
1:C:3268:ILE:HD11	1:C:3319:LEU:HD11	1.67	0.77
1:A:1079:ASN:ND2	2:A:179:NAG:H2	2.00	0.77
1:D:4359:ILE:HD13	3:D:4:NLX:H71	1.67	0.76
1:F:6097:LEU:HD22	3:F:6:NLX:C19	2.13	0.76
1:K:5395:LEU:HB3	1:K:5550:LEU:HD21	1.66	0.76
1:D:4304:LEU:HG	3:D:4:NLX:H201	1.67	0.76
1:L:6304:LEU:HD22	3:L:6:NLX:H102	1.67	0.76
1:G:1290:THR:OG1	1:G:1293:GLU:HG3	1.86	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:3512:GLU:CD	1:I:3512:GLU:H	1.86	0.76
1:D:4538:LYS:HD3	1:D:4541:ASP:OD1	1.86	0.76
1:D:4471:GLU:O	1:D:4475:VAL:HG23	1.85	0.76
1:E:5142:GLY:HA2	3:E:5:N LX:H82	1.67	0.76
1:G:1228:SER:O	1:G:1231:VAL:HG12	1.85	0.76
1:L:6142:GLY:HA2	3:L:6:N LX:H82	1.69	0.75
1:I:3428:VAL:HB	1:I:3429:PRO:HD3	1.68	0.75
1:D:4349:GLY:HA3	1:D:4447:TYR:CZ	2.20	0.75
1:H:2304:LEU:HB3	3:H:2:N LX:C20	2.13	0.75
1:B:2359:ILE:HG13	4:B:7392:HOH:O	1.85	0.75
1:F:6215:VAL:H	1:F:6241:HIS:CD2	2.04	0.75
1:H:2220:GLU:HG2	1:H:2472:LEU:HD21	1.68	0.75
1:H:2215:VAL:H	1:H:2241:HIS:HD2	1.34	0.75
1:I:3353:GLN:NE2	1:I:3465:ILE:H	1.85	0.75
1:K:5304:LEU:HD22	3:K:5:N LX:H102	1.69	0.75
1:K:5382:LEU:HD11	1:K:5391:ILE:HD12	1.69	0.75
1:F:6452:ARG:HB2	1:F:6465:ILE:HG12	1.69	0.75
1:J:4059:PRO:HD3	1:J:4117:LEU:HD12	1.69	0.74
3:C:3:N LX:C17	3:C:3:N LX:C9	2.64	0.74
1:C:3215:VAL:N	1:C:3241:HIS:HD2	1.81	0.74
1:D:4242:ARG:HG2	1:D:4242:ARG:NH1	2.01	0.74
1:H:2176:GLY:HA2	1:H:2189:TRP:HB2	1.69	0.74
1:B:2318:LEU:CG	3:B:2:N LX:H171	2.18	0.74
1:C:3371:GLY:O	1:C:3411:VAL:HA	1.88	0.74
1:H:2371:GLY:HA2	1:H:2414:LYS:HD3	1.68	0.74
1:F:6257:LYS:HA	1:F:6257:LYS:HE3	1.70	0.74
1:B:2372:GLN:O	1:B:2410:THR:HB	1.87	0.74
1:A:1090:ASP:HB3	1:A:1093:ALA:HB3	1.67	0.74
1:B:2234:PRO:O	1:B:2237:LYS:HG2	1.87	0.73
1:F:6242:ARG:HH11	1:F:6242:ARG:HG2	1.54	0.73
1:H:2370:GLU:HG3	1:K:5461:PRO:HG3	1.69	0.73
1:G:1363:LEU:HB3	3:G:1:N LX:H181	1.71	0.73
1:C:3242:ARG:HG2	1:C:3242:ARG:NH1	2.01	0.73
1:I:3498:LYS:HB3	1:I:3514:LEU:HD11	1.70	0.73
1:J:4304:LEU:HG	3:J:4:N LX:H203	1.70	0.73
1:J:4251:LEU:HD11	1:J:4336:GLN:HE22	1.52	0.73
1:F:6353:GLN:NE2	1:F:6465:ILE:H	1.86	0.73
1:G:1428:VAL:HB	1:G:1429:PRO:HD3	1.70	0.73
1:B:2359:ILE:HB	1:B:2360:PRO:CD	2.19	0.73
1:K:5363:LEU:HB2	3:K:5:N LX:H201	1.70	0.73
1:I:3142:GLY:HA2	3:I:3:N LX:H71	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4359:ILE:HB	1:D:4360:PRO:HD3	1.71	0.73
1:D:4304:LEU:HB3	3:D:4:NLX:H201	1.69	0.73
1:G:1215:VAL:H	1:G:1241:HIS:CD2	2.02	0.73
1:L:6358:LEU:HG	1:L:6363:LEU:HD12	1.71	0.72
1:H:2420:LEU:O	1:H:2424:VAL:HG23	1.89	0.72
1:F:6235:LEU:HD12	1:F:6327:LEU:HD12	1.70	0.72
1:C:3143:GLY:HA3	3:C:3:NLX:C15	2.18	0.72
1:B:2304:LEU:HA	3:B:2:NLX:H191	1.71	0.72
1:B:2371:GLY:HA2	1:B:2414:LYS:HD3	1.71	0.72
1:F:6097:LEU:CD2	3:F:6:NLX:H192	2.18	0.72
1:K:5396:ILE:HB	1:K:5397:PRO:HD3	1.69	0.72
1:E:5235:LEU:HD12	1:E:5327:LEU:HA	1.70	0.72
1:J:4260:ASP:OD2	1:J:4263:PRO:HD3	1.89	0.72
1:D:4363:LEU:HB3	3:D:4:NLX:C18	2.18	0.72
1:K:5353:GLN:NE2	1:K:5465:ILE:H	1.87	0.72
1:L:6030:HIS:HB3	1:L:6073:PRO:HA	1.69	0.72
1:B:2083:TYR:CE2	1:B:2108:ILE:HD13	2.25	0.72
1:F:6359:ILE:HB	1:F:6360:PRO:HD3	1.71	0.72
1:E:5308:LEU:HD21	1:E:5367:PRO:HG3	1.70	0.72
1:A:1095:GLN:O	1:A:1099:GLU:HG3	1.90	0.72
1:D:4354:GLU:O	1:D:4468:HIS:HB2	1.90	0.72
1:C:3249:VAL:HG23	1:C:3251:LEU:H	1.55	0.72
1:E:5308:LEU:HD21	1:E:5367:PRO:CG	2.20	0.71
1:A:1237:LYS:HG2	1:A:1238:ASN:ND2	2.05	0.71
3:C:3:NLX:C9	3:C:3:NLX:C20	2.68	0.71
1:E:5491:ARG:HG2	4:E:7516:HOH:O	1.89	0.71
1:H:2048:ALA:HB3	1:H:2123:THR:HG23	1.72	0.71
1:H:2227:VAL:O	1:H:2231:VAL:HG23	1.91	0.71
1:L:6255:LEU:HD23	1:L:6318:LEU:HD13	1.73	0.71
1:F:6034:LEU:HD12	1:F:6079:ASN:HD22	1.53	0.71
1:A:1104:ARG:CZ	1:A:1153:ASP:HB2	2.20	0.71
1:B:2355:PHE:CE2	1:B:2359:ILE:HG21	2.25	0.71
1:G:1104:ARG:HB3	1:G:1104:ARG:HH11	1.55	0.71
1:K:5359:ILE:HG23	3:K:5:NLX:H152	1.71	0.71
1:A:1527:LEU:HD11	1:A:1533:THR:CG2	2.19	0.71
1:B:2353:GLN:NE2	1:B:2465:ILE:H	1.88	0.71
1:A:1319:LEU:H	1:A:1319:LEU:HD12	1.56	0.70
1:E:5255:LEU:HD23	1:E:5318:LEU:HD13	1.74	0.70
1:H:2121:ILE:HD13	1:H:2166:VAL:HG22	1.73	0.70
1:E:5304:LEU:HB3	3:E:5:NLX:C18	2.21	0.70
1:K:5024:PRO:HD3	1:K:5037:PHE:CD1	2.27	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:2158:ALA:HB2	1:H:2165:VAL:HG23	1.72	0.70
1:A:1313:ARG:HG2	1:A:1386:TYR:CE2	2.27	0.70
1:D:4508:ASN:HD21	1:D:4510:ASN:HB2	1.57	0.70
1:C:3319:LEU:HA	4:C:7152:HOH:O	1.92	0.70
4:B:7643:HOH:O	1:E:5092:LYS:HD2	1.91	0.70
1:E:5363:LEU:HB2	3:E:5:NLX:H201	1.74	0.70
1:H:2359:ILE:HD13	3:H:2:NLX:H71	1.72	0.70
1:L:6029:VAL:HG23	1:L:6204:ASN:OD1	1.92	0.70
1:L:6550:LEU:HA	1:L:6553:LYS:NZ	2.05	0.70
1:A:1215:VAL:H	1:A:1241:HIS:CD2	2.04	0.69
1:E:5089:GLN:HB2	1:E:5146:VAL:HG12	1.72	0.69
1:I:3215:VAL:H	1:I:3241:HIS:HD2	1.38	0.69
1:D:4161:GLU:OE2	1:D:4498:LYS:HA	1.92	0.69
1:D:4428:VAL:HB	1:D:4429:PRO:HD3	1.73	0.69
1:B:2079:ASN:ND2	2:B:279:NAG:C1	2.55	0.69
1:G:1023:PRO:HB2	1:G:1034:LEU:HD21	1.74	0.69
1:L:6373:LEU:HB2	1:L:6414:LYS:HB3	1.75	0.69
1:A:1349:GLY:HA3	1:A:1447:TYR:CE1	2.27	0.69
1:K:5082:SER:HB2	4:K:7929:HOH:O	1.92	0.69
1:D:4343:THR:HA	4:D:7962:HOH:O	1.92	0.69
1:I:3491:ARG:HA	1:I:3494:LYS:HD3	1.74	0.69
1:G:1404:LEU:HB3	1:G:1413:LYS:HG3	1.74	0.69
1:H:2258:LYS:HD2	4:H:7424:HOH:O	1.92	0.69
1:G:1385:SER:O	1:G:1389:VAL:HG22	1.93	0.69
1:L:6262:LYS:O	1:L:6266:GLU:HG2	1.93	0.69
1:I:3242:ARG:HH11	1:I:3242:ARG:HG2	1.58	0.69
1:L:6260:ASP:HA	4:L:7557:HOH:O	1.93	0.69
1:B:2227:VAL:O	1:B:2231:VAL:HG23	1.91	0.69
1:L:6359:ILE:HB	1:L:6360:PRO:HD3	1.73	0.69
1:L:6215:VAL:N	1:L:6241:HIS:HD2	1.91	0.69
1:G:1429:PRO:O	1:G:1433:VAL:HG23	1.92	0.69
1:L:6355:PHE:CE1	1:L:6360:PRO:HG3	2.27	0.69
1:F:6395:LEU:HB3	1:F:6550:LEU:HD21	1.73	0.69
1:L:6257:LYS:HE2	1:L:6316:GLN:NE2	2.08	0.69
1:C:3404:LEU:HD22	1:C:3413:LYS:O	1.92	0.69
1:E:5264:LEU:HD13	1:E:5316:GLN:HG3	1.73	0.69
1:I:3217:ILE:O	1:I:3217:ILE:HG13	1.92	0.69
1:K:5420:LEU:HD12	1:K:5547:TRP:HZ2	1.58	0.69
1:C:3132:ARG:HB3	1:C:3211:ASN:HB2	1.74	0.69
1:A:1527:LEU:HD11	1:A:1533:THR:HG22	1.74	0.69
1:G:1304:LEU:CD1	1:G:1318:LEU:HD23	2.23	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3057:LYS:HD3	1:C:3063:LEU:HD11	1.75	0.69
3:C:3:NLX:C10	3:C:3:NLX:C14	2.71	0.68
1:C:3370:GLU:HG3	1:D:4461:PRO:HG3	1.73	0.68
1:C:3527:LEU:HD11	1:C:3533:THR:HG22	1.75	0.68
1:L:6371:GLY:O	1:L:6411:VAL:HA	1.94	0.68
1:C:3428:VAL:HB	1:C:3429:PRO:HD3	1.74	0.68
1:K:5456:SER:HB3	1:K:5460:LYS:HD3	1.75	0.68
1:G:1156:ALA:HB3	4:G:7720:HOH:O	1.91	0.68
1:H:2460:LYS:HG2	4:H:7161:HOH:O	1.94	0.68
1:C:3236:ALA:HA	1:C:3239:LEU:HD12	1.76	0.68
1:J:4334:GLU:O	1:J:4338:GLU:HG2	1.92	0.68
1:L:6550:LEU:HA	1:L:6553:LYS:HZ3	1.56	0.68
1:C:3290:THR:OG1	1:C:3293:GLU:HG3	1.94	0.68
1:H:2221:SER:CB	3:H:2:NLX:O1	2.42	0.68
1:G:1391:ILE:HA	4:G:8113:HOH:O	1.92	0.68
1:K:5351:ASN:HB3	1:K:5466:GLY:O	1.94	0.68
1:H:2363:LEU:HD13	3:H:2:NLX:C10	2.23	0.68
1:D:4260:ASP:OD1	1:D:4263:PRO:HD3	1.94	0.68
1:I:3088:THR:HG22	1:I:3295:LEU:HD13	1.76	0.68
1:F:6024:PRO:HG3	1:F:6037:PHE:CE1	2.28	0.68
1:G:1417:PHE:O	1:G:1420:LEU:HB3	1.95	0.67
1:B:2486:SER:O	1:B:2490:ILE:HG13	1.94	0.67
1:L:6545:ALA:O	1:L:6548:THR:HG22	1.95	0.67
1:L:6271:THR:HG22	1:L:6297:THR:HG23	1.76	0.67
1:J:4525:GLY:HA2	1:J:4537:GLN:HG2	1.76	0.67
1:A:1372:GLN:HB2	1:A:1410:THR:HG22	1.75	0.67
1:B:2174:ILE:HG13	4:B:7012:HOH:O	1.95	0.67
1:A:1385:SER:O	1:A:1389:VAL:HG22	1.95	0.67
1:F:6353:GLN:HE22	1:F:6465:ILE:H	1.40	0.67
1:L:6254:VAL:HG22	1:L:6318:LEU:HD12	1.75	0.67
1:F:6220:GLU:HG2	1:F:6472:LEU:HD21	1.77	0.67
1:H:2386:TYR:N	1:H:2387:PRO:HD2	2.09	0.67
1:F:6174:ILE:HG13	4:F:7076:HOH:O	1.95	0.67
1:A:1376:LYS:HD3	1:F:6462:LYS:CE	2.24	0.67
1:K:5498:LYS:HG2	1:K:5502:ASN:HD21	1.60	0.67
1:F:6043:PHE:HA	4:F:7849:HOH:O	1.94	0.67
1:L:6087:CYS:HB3	4:L:7703:HOH:O	1.95	0.67
1:D:4358:LEU:O	1:D:4363:LEU:HD12	1.95	0.67
1:J:4303:PHE:CZ	1:J:4319:LEU:HD21	2.29	0.67
1:A:1363:LEU:CD2	3:A:1:NLX:H181	2.25	0.67
1:K:5290:THR:OG1	1:K:5293:GLU:HG3	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:6097:LEU:HB2	3:F:6:NLX:H192	1.77	0.67
1:I:3317:PRO:HG2	3:I:3:NLX:C19	2.25	0.67
1:J:4215:VAL:H	1:J:4241:HIS:CD2	2.11	0.67
1:I:3324:ASP:OD1	1:I:3326:MET:HB2	1.94	0.67
1:H:2186:ARG:HB3	1:H:2324:ASP:HB2	1.77	0.67
1:E:5125:ALA:HB1	1:E:5131:ASN:ND2	2.10	0.67
1:C:3227:VAL:O	1:C:3231:VAL:HG23	1.94	0.67
1:E:5242:ARG:HH11	1:E:5242:ARG:HG3	1.61	0.66
1:L:6429:PRO:O	1:L:6433:VAL:HG23	1.95	0.66
1:A:1363:LEU:HD13	3:A:1:NLX:C10	2.24	0.66
1:B:2304:LEU:HA	3:B:2:NLX:C19	2.25	0.66
1:H:2083:TYR:CE2	1:H:2108:ILE:HD13	2.31	0.66
1:A:1363:LEU:HB3	3:A:1:NLX:H181	1.77	0.66
1:B:2371:GLY:HA3	1:E:5371:GLY:HA3	1.77	0.66
1:D:4409:ASP:HB3	1:D:4412:LYS:HB2	1.78	0.66
1:K:5221:SER:HB2	3:K:5:NLX:O3	1.95	0.66
1:G:1142:GLY:HA2	3:G:1:NLX:H152	1.76	0.66
1:G:1146:VAL:HG21	3:G:1:NLX:H162	1.77	0.66
1:L:6141:GLY:N	4:L:7115:HOH:O	2.22	0.66
1:E:5145:MET:HB2	1:E:5304:LEU:HD11	1.76	0.66
1:J:4132:ARG:HH12	1:J:4206:ALA:HB1	1.59	0.66
1:H:2498:LYS:HG2	1:H:2514:LEU:HD11	1.76	0.66
1:F:6411:VAL:HG23	4:F:7705:HOH:O	1.94	0.66
1:F:6414:LYS:HD2	1:F:6415:ASP:N	2.11	0.66
1:L:6216:THR:HG23	1:L:6242:ARG:HB2	1.78	0.66
1:F:6143:GLY:N	3:F:6:NLX:H82	2.11	0.66
1:J:4221:SER:OG	1:J:4222:ALA:N	2.28	0.66
1:L:6395:LEU:HD22	1:L:6550:LEU:HD11	1.77	0.66
1:F:6258:LYS:O	1:F:6258:LYS:HE2	1.95	0.66
1:L:6083:TYR:CE2	1:L:6108:ILE:HD13	2.31	0.66
1:L:6375:GLN:HE22	1:L:6401:GLU:HA	1.61	0.66
1:J:4396:ILE:HB	1:J:4397:PRO:HD3	1.77	0.66
1:E:5409:ASP:OD2	1:E:5411:VAL:HB	1.96	0.66
1:C:3498:LYS:HB3	1:C:3514:LEU:HD11	1.75	0.66
1:I:3412:LYS:O	1:I:3416:LEU:HG	1.95	0.66
1:J:4191:HIS:O	1:J:4195:VAL:HG23	1.95	0.66
1:D:4303:PHE:O	1:D:4304:LEU:HB2	1.95	0.66
1:E:5304:LEU:HD21	1:E:5318:LEU:CD2	2.26	0.66
1:J:4364:MET:SD	3:J:4:NLX:H72	2.35	0.66
1:G:1146:VAL:CG2	3:G:1:NLX:H162	2.26	0.66
1:L:6024:PRO:HA	4:L:7722:HOH:O	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1232:LEU:HD23	1:A:1341:PHE:HB3	1.78	0.66
1:K:5104:ARG:NH1	1:K:5153:ASP:HB2	2.10	0.66
1:C:3407:THR:HG21	1:C:3412:LYS:NZ	2.11	0.66
1:G:1220:GLU:HA	1:G:1246:GLU:O	1.97	0.65
1:A:1428:VAL:HB	1:A:1429:PRO:HD3	1.78	0.65
1:K:5218:PHE:HB2	1:K:5244:ILE:HB	1.77	0.65
1:E:5134:PRO:HG2	1:E:5163:VAL:HG12	1.78	0.65
3:F:6:NLX:O4	4:F:7502:HOH:O	2.13	0.65
1:A:1358:LEU:HG	1:A:1363:LEU:CD1	2.26	0.65
1:E:5371:GLY:O	1:E:5414:LYS:HD3	1.97	0.65
1:I:3398:GLU:HG3	4:I:8065:HOH:O	1.95	0.65
1:J:4237:LYS:HE2	1:J:4238:ASN:HD21	1.59	0.65
1:J:4304:LEU:HG	3:J:4:NLX:C20	2.26	0.65
1:G:1363:LEU:HD13	3:G:1:NLX:H102	1.78	0.65
1:E:5395:LEU:HB3	1:E:5550:LEU:HD11	1.78	0.65
1:I:3447:TYR:HB3	1:I:3517:TRP:CZ2	2.31	0.65
1:D:4395:LEU:HD13	1:D:4550:LEU:HG	1.78	0.65
1:D:4257:LYS:HZ1	1:D:4316:GLN:HG3	1.60	0.65
1:I:3125:ALA:HB2	1:I:3133:LEU:HD11	1.79	0.65
1:J:4549:ASN:HB2	4:J:8096:HOH:O	1.95	0.65
1:G:1276:THR:HG22	1:G:1282:MET:SD	2.36	0.65
1:L:6139:ILE:HG22	4:L:7115:HOH:O	1.96	0.65
1:J:4104:ARG:NH1	1:J:4153:ASP:HB2	2.12	0.65
1:E:5149:ALA:HB1	1:E:5167:THR:HB	1.79	0.65
1:C:3357:TRP:O	1:C:3360:PRO:HD2	1.96	0.65
1:B:2359:ILE:HG23	3:B:2:NLX:C8	2.25	0.65
1:A:1086:MET:HE2	1:A:1110:LEU:HD12	1.77	0.65
1:D:4330:LYS:HG3	1:D:4335:LEU:HG	1.78	0.65
1:I:3364:MET:SD	3:I:3:NLX:H162	2.37	0.65
1:J:4429:PRO:O	1:J:4433:VAL:HG23	1.97	0.65
1:L:6024:PRO:HG3	1:L:6037:PHE:CE1	2.31	0.65
1:E:5290:THR:OG1	1:E:5293:GLU:HG3	1.95	0.65
1:E:5279:SER:HA	1:E:5282:MET:HE3	1.77	0.65
1:A:1251:LEU:HD11	1:A:1336:GLN:NE2	2.02	0.65
1:H:2426:PHE:O	1:H:2429:PRO:HD2	1.97	0.65
1:J:4404:LEU:HD13	1:J:4413:LYS:HB3	1.77	0.65
1:G:1444:THR:O	1:G:1519:GLU:HG2	1.97	0.64
1:B:2456:SER:HB3	1:B:2460:LYS:HD3	1.78	0.64
1:J:4461:PRO:HG2	1:J:4464:VAL:HG23	1.79	0.64
1:C:3313:ARG:HG2	1:C:3386:TYR:CE2	2.32	0.64
1:J:4427:GLY:O	1:J:4431:VAL:HG23	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:6252:THR:HG23	1:F:6425:MET:O	1.96	0.64
1:A:1353:GLN:HE22	1:A:1465:ILE:H	1.45	0.64
1:E:5258:LYS:HD2	1:E:5258:LYS:O	1.97	0.64
1:F:6456:SER:HB3	1:F:6460:LYS:HD3	1.78	0.64
1:F:6343:THR:HB	1:F:6442:ALA:HB2	1.80	0.64
1:J:4227:VAL:O	1:J:4231:VAL:HG23	1.97	0.64
1:F:6221:SER:OG	3:F:6:NLX:H72	1.98	0.64
1:C:3296:GLU:HG2	1:D:4296:GLU:OE1	1.98	0.64
1:D:4079:ASN:HB2	2:D:479:NAG:H82	1.80	0.64
1:E:5464:VAL:C	1:E:5465:ILE:HD12	2.17	0.64
1:G:1218:PHE:CB	1:G:1244:ILE:HB	2.27	0.64
1:H:2090:ASP:HB3	1:H:2093:ALA:HB3	1.79	0.64
1:I:3296:GLU:O	1:I:3300:LYS:HG3	1.97	0.64
1:E:5486:SER:O	1:E:5490:ILE:HG13	1.98	0.64
1:I:3486:SER:O	1:I:3490:ILE:HG13	1.98	0.64
1:E:5359:ILE:HG23	3:E:5:NLX:H152	1.80	0.64
1:F:6540:LYS:HD3	1:F:6543:GLU:OE1	1.97	0.64
1:J:4130:LYS:HE2	1:J:4132:ARG:NE	2.13	0.63
1:L:6414:LYS:HE2	1:L:6415:ASP:OD2	1.97	0.63
1:J:4098:SER:O	1:J:4102:THR:HG22	1.97	0.63
1:G:1435:ARG:NH1	1:G:1544:VAL:HG11	2.12	0.63
1:K:5311:ASP:HB3	1:K:5314:GLU:HG2	1.80	0.63
1:D:4251:LEU:HD21	1:D:4333:GLU:HG3	1.80	0.63
1:I:3452:ARG:HB2	1:I:3465:ILE:HG12	1.79	0.63
1:G:1215:VAL:N	1:G:1241:HIS:HD2	1.91	0.63
1:G:1519:GLU:O	1:G:1521:ASN:N	2.31	0.63
1:A:1435:ARG:NH1	1:A:1544:VAL:HG11	2.14	0.63
1:F:6311:ASP:OD1	1:F:6313:ARG:HB2	1.98	0.63
1:F:6258:LYS:HE2	1:F:6258:LYS:N	2.13	0.63
1:G:1140:HIS:HD2	1:G:1141:GLY:O	1.81	0.63
1:E:5340:ASN:ND2	1:E:5342:HIS:H	1.96	0.63
1:F:6258:LYS:H	1:F:6258:LYS:HE2	1.64	0.63
1:L:6051:LEU:HD13	1:L:6083:TYR:CE1	2.33	0.63
1:A:1264:LEU:HG	1:A:1316:GLN:HG2	1.80	0.63
1:I:3142:GLY:CA	3:I:3:NLX:H71	2.29	0.63
1:F:6478:ALA:HB3	1:F:6479:PRO:HD3	1.79	0.63
1:A:1216:THR:HG23	1:A:1242:ARG:HB2	1.80	0.63
1:D:4396:ILE:HB	1:D:4397:PRO:HD3	1.80	0.63
1:E:5215:VAL:H	1:E:5241:HIS:HD2	1.47	0.63
1:K:5149:ALA:HB2	1:K:5169:GLN:HG3	1.80	0.63
1:K:5526:TYR:HD2	1:K:5537:GLN:O	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:5523:LYS:O	1:E:5538:LYS:HE3	1.98	0.63
1:A:1304:LEU:CD1	1:A:1318:LEU:HD23	2.29	0.63
1:G:1279:SER:O	1:G:1283:VAL:HG23	1.98	0.63
1:B:2149:ALA:HB2	1:B:2169:GLN:HG3	1.80	0.63
1:E:5351:ASN:OD1	1:E:5449:PHE:HB3	1.98	0.63
1:H:2526:TYR:CE1	1:H:2539:LEU:HD13	2.34	0.63
1:F:6138:TRP:CZ3	1:F:6219:GLY:HA2	2.34	0.63
1:J:4079:ASN:HD21	2:J:479:NAG:H5	1.63	0.63
1:D:4126:ASP:H	1:D:4131:ASN:ND2	1.96	0.63
1:H:2235:LEU:HD12	1:H:2327:LEU:HA	1.80	0.63
1:D:4461:PRO:HG2	1:D:4464:VAL:HG23	1.80	0.63
1:G:1409:ASP:HB3	1:G:1412:LYS:HB2	1.80	0.63
1:G:1092:LYS:NZ	1:L:6302:LYS:HB2	2.13	0.63
1:K:5324:ASP:OD1	1:K:5326:MET:HB2	1.99	0.63
1:J:4407:THR:HG21	1:J:4412:LYS:HD2	1.81	0.63
3:C:3:NLX:C13	3:C:3:NLX:C9	2.76	0.62
1:K:5467:ASP:OD1	1:K:5468:HIS:N	2.30	0.62
1:A:1363:LEU:CD1	3:A:1:NLX:H101	2.28	0.62
1:A:1386:TYR:N	1:A:1387:PRO:HD2	2.14	0.62
1:L:6523:LYS:HB3	1:L:6537:GLN:OE1	1.98	0.62
1:D:4423:ASP:OD1	1:D:4540:LYS:HE2	1.99	0.62
1:J:4354:GLU:O	1:J:4468:HIS:HB2	1.99	0.62
1:C:3351:ASN:ND2	1:C:3449:PHE:HB3	2.14	0.62
1:I:3220:GLU:HG2	4:I:7760:HOH:O	1.99	0.62
1:E:5188:ASN:O	1:E:5192:LEU:HG	1.99	0.62
1:E:5089:GLN:OE1	1:E:5146:VAL:HB	1.99	0.62
1:D:4145:MET:HG3	1:D:4304:LEU:HD11	1.80	0.62
1:F:6097:LEU:HD13	3:F:6:NLX:H191	1.82	0.62
1:A:1359:ILE:HG23	3:A:1:NLX:H71	1.82	0.62
1:H:2463:THR:HG23	4:H:7113:HOH:O	1.98	0.62
1:E:5311:ASP:O	1:E:5314:GLU:HG2	1.99	0.62
1:C:3324:ASP:OD1	1:C:3326:MET:HB2	1.98	0.62
3:C:3:NLX:H102	3:C:3:NLX:C20	2.30	0.62
1:K:5464:VAL:C	1:K:5465:ILE:HD12	2.20	0.62
1:I:3234:PRO:O	1:I:3237:LYS:HE3	1.98	0.62
1:J:4034:LEU:CD1	2:J:479:NAG:H82	2.30	0.62
1:I:3358:LEU:O	1:I:3363:LEU:HD12	1.99	0.62
1:H:2304:LEU:HD13	3:H:2:NLX:H171	1.80	0.62
1:F:6304:LEU:HD22	3:F:6:NLX:H101	1.81	0.62
1:A:1030:HIS:HB3	1:A:1073:PRO:HA	1.81	0.62
1:K:5403:TYR:O	1:K:5416:LEU:HD13	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1471:GLU:O	1:G:1475:VAL:HG23	1.99	0.62
1:F:6097:LEU:HD11	1:F:6101:PHE:CE2	2.35	0.62
1:L:6363:LEU:HB3	3:L:6:N LX:H201	1.79	0.62
1:K:5220:GLU:O	1:K:5221:SER:HB3	1.99	0.62
1:G:1417:PHE:CD1	1:G:1420:LEU:HD23	2.34	0.62
1:I:3381:LEU:HD23	1:J:4459:MET:HG2	1.82	0.62
1:J:4251:LEU:HD11	1:J:4336:GLN:NE2	2.14	0.61
1:A:1086:MET:HE2	1:A:1110:LEU:HB2	1.82	0.61
1:A:1279:SER:O	1:A:1283:VAL:HG23	2.00	0.61
1:K:5428:VAL:HB	1:K:5429:PRO:HD3	1.81	0.61
1:D:4349:GLY:HA3	1:D:4447:TYR:CE1	2.35	0.61
1:A:1409:ASP:HB3	1:A:1412:LYS:HB2	1.82	0.61
1:I:3302:LYS:HD2	1:J:4092:LYS:HD2	1.80	0.61
1:A:1308:LEU:HD11	1:A:1367:PRO:HG3	1.82	0.61
1:G:1395:LEU:HB3	1:G:1550:LEU:HD11	1.83	0.61
1:F:6144:LEU:HB3	1:F:6177:PHE:CE2	2.35	0.61
1:G:1373:LEU:O	1:G:1413:LYS:HD2	1.99	0.61
1:C:3268:ILE:HG12	1:C:3301:MET:HE2	1.81	0.61
1:L:6447:TYR:CD2	1:L:6447:TYR:C	2.74	0.61
1:B:2024:PRO:HG3	1:B:2037:PHE:CE1	2.35	0.61
1:A:1423:ASP:O	1:A:1428:VAL:HG23	2.01	0.61
1:J:4386:TYR:N	1:J:4387:PRO:HD2	2.16	0.61
1:F:6140:HIS:HD2	1:F:6141:GLY:O	1.83	0.61
1:J:4032:LYS:HB2	1:J:4077:VAL:HA	1.82	0.61
1:H:2264:LEU:HD22	1:H:2316:GLN:HE21	1.63	0.61
3:D:4:N LX:O4	3:D:4:N LX:H203	2.00	0.61
1:G:1302:LYS:CG	1:L:6092:LYS:NZ	2.63	0.61
1:G:1303:PHE:HB3	1:G:1304:LEU:HD22	1.81	0.61
1:L:6257:LYS:HE2	1:L:6316:GLN:CD	2.21	0.61
1:B:2174:ILE:CD1	1:B:2298:THR:HG22	2.29	0.61
1:K:5104:ARG:CZ	1:K:5153:ASP:HB2	2.30	0.61
1:K:5218:PHE:CB	1:K:5244:ILE:HB	2.30	0.61
1:J:4231:VAL:O	1:J:4341:PHE:HB2	1.99	0.61
1:A:1114:GLU:HG3	1:A:1291:GLU:OE2	2.00	0.61
1:I:3258:LYS:H	1:I:3258:LYS:HE2	1.65	0.61
1:L:6363:LEU:HB3	3:L:6:N LX:H162	1.82	0.61
1:I:3144:LEU:HD12	1:I:3320:GLY:HA2	1.82	0.61
1:J:4081:THR:OG1	2:J:479:NAG:H5	2.00	0.61
1:J:4074:TRP:CE2	1:J:4078:LYS:HE2	2.36	0.61
1:G:1357:TRP:CE3	1:G:1460:LYS:HD3	2.35	0.61
1:G:1452:ARG:HB2	1:G:1465:ILE:HG13	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3364:MET:SD	3:C:3:N LX:C18	2.87	0.61
1:K:5258:LYS:HD2	1:K:5258:LYS:N	2.03	0.61
1:I:3352:LYS:HE3	1:I:3450:GLN:NE2	2.15	0.61
1:B:2104:ARG:HG2	1:B:2104:ARG:HH11	1.66	0.61
1:C:3495:MET:HG3	1:C:3514:LEU:HD22	1.82	0.61
1:B:2498:LYS:HG2	1:B:2514:LEU:HD11	1.82	0.61
1:C:3478:ALA:N	1:C:3479:PRO:CD	2.63	0.61
1:I:3363:LEU:HD13	4:I:7519:HOH:O	2.01	0.61
1:G:1355:PHE:CE1	1:G:1360:PRO:HG3	2.35	0.61
1:L:6024:PRO:HG3	1:L:6037:PHE:CZ	2.36	0.61
1:B:2024:PRO:HG3	1:B:2037:PHE:CZ	2.36	0.61
1:B:2464:VAL:CG2	1:E:5370:GLU:HG3	2.31	0.61
1:E:5524:GLU:OE2	1:E:5538:LYS:HD3	2.01	0.61
1:F:6047:VAL:HG21	1:F:6155:LEU:HD23	1.83	0.61
1:F:6527:LEU:HD11	1:F:6533:THR:HG22	1.82	0.61
1:K:5366:TYR:HB3	1:K:5368:LEU:HD13	1.81	0.60
1:A:1371:GLY:O	1:A:1414:LYS:HD3	2.00	0.60
1:J:4023:PRO:HB2	1:J:4034:LEU:HD21	1.82	0.60
1:G:1452:ARG:HG2	1:G:1452:ARG:HH11	1.66	0.60
1:D:4421:ILE:HG22	1:D:4425:MET:HE2	1.83	0.60
1:J:4302:LYS:NZ	1:J:4302:LYS:HB3	2.16	0.60
1:G:1456:SER:HB3	1:G:1460:LYS:HE3	1.82	0.60
1:K:5284:HIS:O	1:K:5288:GLN:HG3	2.00	0.60
1:F:6417:PHE:O	1:F:6420:LEU:HB3	2.02	0.60
1:F:6097:LEU:HD11	1:F:6101:PHE:CD2	2.36	0.60
1:K:5304:LEU:HD22	3:K:5:N LX:C10	2.32	0.60
1:A:1257:LYS:HD2	1:A:1320:GLY:H	1.66	0.60
1:A:1304:LEU:HB3	3:A:1:N LX:C20	2.31	0.60
1:F:6324:ASP:OD1	1:F:6326:MET:N	2.32	0.60
1:E:5353:GLN:NE2	1:E:5465:ILE:H	1.99	0.60
1:L:6478:ALA:HB3	1:L:6479:PRO:HD3	1.82	0.60
1:L:6104:ARG:HH11	1:L:6104:ARG:HG2	1.64	0.60
1:E:5452:ARG:NE	1:E:5462:LYS:HA	2.16	0.60
1:E:5266:GLU:O	1:E:5270:ILE:HG13	2.00	0.60
1:F:6355:PHE:CE1	1:F:6360:PRO:HG3	2.36	0.60
1:A:1145:MET:HB2	1:A:1304:LEU:HD21	1.83	0.60
1:L:6428:VAL:HB	1:L:6429:PRO:HD3	1.83	0.60
1:A:1244:ILE:HG12	1:A:1347:MET:HB3	1.84	0.60
1:G:1064:ARG:NH1	1:G:1294:LEU:HD11	2.15	0.60
1:E:5330:LYS:HB3	1:E:5334:GLU:OE2	2.01	0.60
1:F:6083:TYR:CE2	1:F:6108:ILE:HD13	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1308:LEU:HD21	1:G:1367:PRO:CG	2.32	0.60
1:E:5292:GLU:O	1:E:5296:GLU:HG3	2.02	0.60
1:K:5487:GLU:O	1:K:5491:ARG:HG3	2.02	0.60
1:L:6174:ILE:HG13	4:L:7009:HOH:O	2.01	0.60
1:L:6086:MET:HG3	1:L:6112:LEU:HD23	1.82	0.60
1:E:5487:GLU:O	1:E:5491:ARG:HG3	2.01	0.60
1:I:3395:LEU:HB3	1:I:3550:LEU:HD11	1.84	0.60
1:I:3284:HIS:O	1:I:3288:GLN:HG2	2.02	0.60
1:J:4468:HIS:CD2	3:J:4:NLX:H21	2.36	0.60
1:I:3352:LYS:HG3	1:I:3353:GLN:HG3	1.82	0.60
1:H:2257:LYS:HE3	1:H:2316:GLN:HE22	1.66	0.60
1:K:5341:PHE:HD2	1:K:5341:PHE:H	1.50	0.60
1:L:6538:LYS:HB3	1:L:6541:ASP:HB2	1.82	0.60
1:L:6324:ASP:OD1	1:L:6326:MET:HB2	2.02	0.60
1:L:6086:MET:CE	1:L:6110:LEU:HB2	2.31	0.60
1:H:2536:ALA:O	1:H:2537:GLN:HG3	2.01	0.60
1:L:6409:ASP:HB3	1:L:6412:LYS:HB2	1.82	0.60
1:C:3332:PRO:O	1:C:3336:GLN:HG3	2.02	0.60
1:F:6136:MET:HB3	1:F:6218:PHE:CE1	2.37	0.60
1:I:3464:VAL:CG2	1:J:4370:GLU:HG3	2.32	0.60
1:F:6351:ASN:HB3	1:F:6466:GLY:O	2.02	0.60
1:B:2402:LYS:HG2	1:B:2546:PHE:CE1	2.37	0.60
1:C:3083:TYR:CE2	1:C:3108:ILE:HD13	2.37	0.59
1:B:2255:LEU:HD23	1:B:2318:LEU:CD1	2.33	0.59
1:L:6145:MET:HE1	1:L:6303:PHE:CD1	2.38	0.59
1:L:6262:LYS:HB3	1:L:6263:PRO:HD3	1.82	0.59
1:D:4025:VAL:HG22	1:D:4034:LEU:HD23	1.82	0.59
1:B:2216:THR:HG23	1:B:2242:ARG:CB	2.32	0.59
1:F:6029:VAL:HG13	4:F:7744:HOH:O	2.02	0.59
1:E:5104:ARG:HD2	4:E:7316:HOH:O	2.01	0.59
1:K:5091:PRO:HG3	1:K:5112:LEU:HD21	1.84	0.59
1:F:6186:ARG:HD3	1:F:6324:ASP:O	2.02	0.59
1:F:6220:GLU:HA	1:F:6246:GLU:O	2.03	0.59
1:J:4134:PRO:HG2	1:J:4163:VAL:HG12	1.83	0.59
1:I:3180:THR:HG23	1:I:3185:SER:HB3	1.84	0.59
1:B:2317:PRO:HB2	3:B:2:NLX:C19	2.31	0.59
1:H:2370:GLU:C	1:H:2372:GLN:H	2.03	0.59
1:A:1359:ILE:HB	1:A:1360:PRO:HD3	1.84	0.59
1:L:6493:SER:O	1:L:6497:MET:HG3	2.01	0.59
1:I:3538:LYS:HE2	1:I:3541:ASP:OD1	2.02	0.59
1:I:3064:ARG:HD3	1:I:3065:PHE:CZ	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1477:GLY:HA2	1:A:1493:SER:OG	2.03	0.59
1:B:2104:ARG:HG2	1:B:2104:ARG:NH1	2.17	0.59
1:D:4260:ASP:OD1	1:D:4262:LYS:HB3	2.01	0.59
1:B:2512:GLU:HB3	4:B:7018:HOH:O	2.01	0.59
1:E:5396:ILE:HB	1:E:5397:PRO:HD3	1.84	0.59
1:H:2379:MET:HG2	1:H:2396:ILE:HG22	1.83	0.59
1:I:3462:LYS:NZ	1:J:4376:LYS:NZ	2.50	0.59
1:E:5125:ALA:HB1	1:E:5131:ASN:HD22	1.66	0.59
1:E:5375:GLN:NE2	1:E:5400:THR:HG22	2.18	0.59
1:L:6048:ALA:HB3	1:L:6123:THR:HG23	1.85	0.59
1:A:1381:LEU:HD21	1:F:6459:MET:HB3	1.85	0.59
1:K:5119:LEU:O	1:K:5119:LEU:HD12	2.02	0.59
1:K:5395:LEU:HD21	1:K:5553:LYS:HB2	1.83	0.59
1:J:4027:ASP:OD1	1:J:4032:LYS:HD3	2.03	0.59
1:I:3478:ALA:N	1:I:3479:PRO:CD	2.66	0.59
1:F:6149:ALA:HB2	1:F:6169:GLN:HG3	1.84	0.59
1:L:6233:SER:O	1:L:6342:HIS:NE2	2.34	0.59
1:A:1478:ALA:N	1:A:1479:PRO:CD	2.65	0.59
1:C:3251:LEU:HD12	1:C:3433:VAL:HG23	1.83	0.59
1:A:1372:GLN:C	1:A:1373:LEU:HD12	2.23	0.59
1:I:3526:TYR:CE2	1:I:3539:LEU:HB2	2.37	0.59
1:L:6420:LEU:CD1	1:L:6547:TRP:CZ2	2.85	0.59
1:D:4038:VAL:HG21	1:D:4049:ILE:HD12	1.85	0.59
1:F:6242:ARG:NH1	1:F:6242:ARG:HG2	2.15	0.59
1:A:1372:GLN:HE21	1:A:1410:THR:HG21	1.67	0.59
1:B:2174:ILE:HG13	1:B:2298:THR:HG22	1.85	0.59
1:F:6135:VAL:HG21	1:F:6205:ILE:HG12	1.85	0.59
1:B:2348:VAL:O	1:B:2446:MET:HA	2.02	0.59
1:B:2386:TYR:N	1:B:2387:PRO:HD2	2.18	0.59
1:J:4304:LEU:HB3	3:J:4:NLX:H203	1.85	0.58
1:L:6105:LYS:HD3	1:L:6106:GLU:CG	2.33	0.58
1:F:6550:LEU:O	1:F:6553:LYS:HB2	2.03	0.58
1:H:2456:SER:HB2	1:H:2460:LYS:HD3	1.85	0.58
1:D:4421:ILE:HG22	1:D:4425:MET:CE	2.33	0.58
1:K:5447:TYR:HA	1:K:5527:LEU:O	2.03	0.58
3:C:3:NLX:C10	3:C:3:NLX:C20	2.82	0.58
1:C:3456:SER:HB3	1:C:3460:LYS:HD3	1.85	0.58
1:A:1309:GLN:NE2	1:A:1310:GLY:N	2.51	0.58
1:G:1313:ARG:HG3	1:G:1313:ARG:HH11	1.67	0.58
1:K:5339:ARG:O	1:K:5339:ARG:HG3	2.02	0.58
1:H:2143:GLY:HA3	3:H:2:NLX:H152	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:5491:ARG:HD2	4:E:7007:HOH:O	2.03	0.58
1:G:1218:PHE:HB3	1:G:1244:ILE:HB	1.84	0.58
1:F:6132:ARG:HB3	1:F:6211:ASN:HB2	1.85	0.58
1:K:5264:LEU:HD13	1:K:5316:GLN:HG3	1.84	0.58
1:G:1339:ARG:HH12	1:G:1436:ASN:HD22	1.50	0.58
1:I:3132:ARG:HB3	1:I:3211:ASN:HB2	1.86	0.58
1:I:3218:PHE:H	1:I:3218:PHE:HD1	1.50	0.58
1:I:3501:ALA:O	1:I:3505:ARG:HG2	2.04	0.58
1:C:3359:ILE:HB	1:C:3360:PRO:HD3	1.86	0.58
1:G:1379:MET:SD	1:G:1397:PRO:HG3	2.44	0.58
1:C:3296:GLU:O	1:C:3300:LYS:HG3	2.04	0.58
1:K:5389:VAL:O	1:K:5390:CYS:HB2	2.03	0.58
1:L:6375:GLN:HE21	1:L:6400:THR:HG22	1.68	0.58
1:C:3309:GLN:HG3	1:D:4096:LEU:HD13	1.83	0.58
1:K:5026:VAL:HG12	1:K:5027:ASP:N	2.17	0.58
1:E:5048:ALA:HB3	1:E:5123:THR:HG23	1.84	0.58
1:F:6215:VAL:N	1:F:6241:HIS:HD2	1.99	0.58
1:B:2528:GLN:O	1:B:2533:THR:HA	2.04	0.58
1:J:4348:VAL:O	1:J:4446:MET:HA	2.04	0.58
1:J:4220:GLU:HG3	1:J:4472:LEU:HD21	1.86	0.58
1:D:4249:VAL:HB	1:D:4433:VAL:HG21	1.85	0.58
1:D:4104:ARG:HD2	4:D:7709:HOH:O	2.01	0.58
1:L:6264:LEU:HD22	1:L:6268:ILE:CD1	2.33	0.58
1:B:2359:ILE:CG1	3:B:2:NLX:H71	2.30	0.58
1:F:6334:GLU:O	1:F:6338:GLU:HG3	2.04	0.58
1:D:4262:LYS:HB3	1:D:4263:PRO:HD3	1.85	0.58
1:G:1435:ARG:O	1:G:1438:ARG:HB3	2.04	0.58
1:L:6026:VAL:CG1	1:L:6207:SER:HB3	2.34	0.58
1:L:6527:LEU:HD11	1:L:6533:THR:HG22	1.85	0.58
1:B:2390:CYS:HB3	4:B:7626:HOH:O	2.02	0.58
1:I:3318:LEU:HB2	4:I:7480:HOH:O	2.04	0.58
1:A:1319:LEU:HD12	1:A:1319:LEU:N	2.18	0.58
1:L:6104:ARG:NH1	1:L:6104:ARG:HG2	2.19	0.58
1:B:2040:LEU:HD13	1:B:2155:LEU:CD1	2.33	0.58
1:K:5133:LEU:HD22	1:K:5162:ASN:O	2.04	0.58
1:J:4333:GLU:CD	1:J:4333:GLU:H	2.07	0.58
1:G:1252:THR:O	1:G:1254:VAL:N	2.36	0.58
1:F:6306:LEU:HD21	1:F:6384:LYS:O	2.04	0.58
1:L:6223:GLY:O	1:L:6227:VAL:HG23	2.04	0.58
1:J:4126:ASP:OD1	1:J:4128:THR:HG23	2.04	0.58
1:C:3257:LYS:HE3	1:C:3322:VAL:CG1	2.33	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:6373:LEU:HD23	1:F:6414:LYS:HA	1.85	0.57
1:J:4034:LEU:HD11	2:J:479:NAG:H82	1.86	0.57
1:I:3456:SER:HB3	1:I:3460:LYS:HD3	1.84	0.57
1:F:6435:ARG:O	1:F:6438:ARG:HB3	2.04	0.57
1:C:3318:LEU:HD21	3:C:3:NLX:H162	1.85	0.57
1:D:4301:MET:HG3	1:D:4303:PHE:CZ	2.39	0.57
1:C:3220:GLU:OE2	1:C:3221:SER:HB2	2.04	0.57
1:A:1342:HIS:CD2	1:A:1342:HIS:N	2.70	0.57
1:E:5142:GLY:HA3	1:E:5146:VAL:O	2.04	0.57
1:H:2372:GLN:NE2	1:H:2410:THR:OG1	2.37	0.57
1:J:4331:THR:HB	1:J:4333:GLU:OE1	2.04	0.57
1:L:6140:HIS:HD2	1:L:6141:GLY:O	1.87	0.57
1:E:5411:VAL:HA	4:E:7302:HOH:O	2.03	0.57
1:G:1521:ASN:HB2	1:G:1522:GLN:NE2	2.19	0.57
1:G:1308:LEU:HD21	1:G:1367:PRO:HG2	1.86	0.57
1:B:2241:HIS:C	1:B:2242:ARG:HD2	2.24	0.57
1:K:5025:VAL:HG22	1:K:5034:LEU:HD23	1.86	0.57
1:D:4363:LEU:HD22	3:D:4:NLX:H102	1.86	0.57
1:J:4142:GLY:C	3:J:4:NLX:H152	2.24	0.57
1:I:3364:MET:HG2	3:I:3:NLX:H201	1.85	0.57
1:G:1104:ARG:CB	1:G:1104:ARG:HH11	2.17	0.57
1:K:5428:VAL:HG13	1:K:5544:VAL:HA	1.86	0.57
1:I:3453:PRO:HD2	1:I:3470:ASP:OD2	2.04	0.57
1:J:4306:LEU:HD22	1:J:4366:TYR:CE1	2.39	0.57
1:J:4140:HIS:CD2	1:J:4147:GLY:HA3	2.40	0.57
1:H:2215:VAL:H	1:H:2241:HIS:CD2	2.18	0.57
1:A:1227:VAL:O	1:A:1231:VAL:HG23	2.04	0.57
1:D:4456:SER:HB3	1:D:4460:LYS:HD3	1.87	0.57
1:J:4493:SER:HB2	4:J:7677:HOH:O	2.04	0.57
1:B:2371:GLY:CA	1:B:2414:LYS:HD3	2.34	0.57
1:F:6024:PRO:HG3	1:F:6037:PHE:CZ	2.40	0.57
1:C:3412:LYS:O	1:C:3416:LEU:HG	2.05	0.57
1:E:5262:LYS:HE2	1:E:5279:SER:OG	2.03	0.57
1:G:1064:ARG:HH11	1:G:1294:LEU:HD11	1.70	0.57
1:L:6420:LEU:HD13	1:L:6547:TRP:HZ2	1.69	0.57
1:F:6095:GLN:O	1:F:6099:GLU:HG3	2.05	0.57
1:H:2371:GLY:CA	1:H:2414:LYS:HD3	2.35	0.57
1:H:2426:PHE:C	1:H:2429:PRO:HD2	2.24	0.57
1:J:4232:LEU:HD23	1:J:4341:PHE:HB3	1.86	0.57
1:A:1358:LEU:HG	1:A:1363:LEU:HD12	1.85	0.57
1:E:5372:GLN:HA	4:E:7302:HOH:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:6348:VAL:O	1:F:6446:MET:HA	2.04	0.57
1:G:1371:GLY:O	1:G:1414:LYS:HD3	2.05	0.57
1:J:4349:GLY:HA3	1:J:4447:TYR:CZ	2.40	0.57
1:C:3437:HIS:HD2	1:C:3444:THR:OG1	1.87	0.57
1:B:2220:GLU:OE2	1:B:2472:LEU:HD11	2.05	0.57
1:L:6104:ARG:NE	1:L:6108:ILE:HD12	2.18	0.57
1:A:1140:HIS:HE1	4:A:7108:HOH:O	1.87	0.57
1:G:1527:LEU:HD11	1:G:1533:THR:HG22	1.87	0.57
1:F:6467:ASP:N	1:F:6470:ASP:OD2	2.38	0.56
1:I:3229:VAL:HG13	1:I:3328:LEU:HD21	1.86	0.56
1:J:4404:LEU:N	1:J:4404:LEU:HD23	2.21	0.56
1:A:1132:ARG:HB3	1:A:1211:ASN:HB2	1.86	0.56
1:F:6359:ILE:HG23	3:F:6:NLX:H152	1.87	0.56
1:I:3242:ARG:NH1	1:I:3242:ARG:HG2	2.20	0.56
1:I:3447:TYR:C	1:I:3447:TYR:CD2	2.78	0.56
1:C:3324:ASP:OD2	1:C:3327:LEU:HB3	2.05	0.56
1:K:5249:VAL:HB	1:K:5433:VAL:HG21	1.86	0.56
1:B:2215:VAL:H	1:B:2241:HIS:HD2	1.53	0.56
1:H:2396:ILE:HB	1:H:2397:PRO:HD3	1.86	0.56
1:E:5386:TYR:N	1:E:5387:PRO:HD2	2.20	0.56
1:K:5138:TRP:CZ3	1:K:5219:GLY:HA2	2.40	0.56
1:D:4309:GLN:NE2	1:D:4309:GLN:C	2.59	0.56
1:C:3138:TRP:CZ3	1:C:3219:GLY:HA2	2.39	0.56
1:E:5190:GLY:O	1:E:5194:GLN:HG3	2.05	0.56
1:C:3401:GLU:OE2	1:C:3405:GLY:HA3	2.04	0.56
1:J:4215:VAL:N	1:J:4241:HIS:HD2	2.03	0.56
1:D:4335:LEU:O	1:D:4340:ASN:ND2	2.24	0.56
1:F:6350:ILE:C	1:F:6351:ASN:HD22	2.07	0.56
1:B:2132:ARG:HB3	1:B:2211:ASN:HB2	1.87	0.56
1:F:6359:ILE:HG12	3:F:6:NLX:H162	1.86	0.56
3:E:5:NLX:O4	3:E:5:NLX:H203	2.06	0.56
1:H:2370:GLU:HG3	1:K:5461:PRO:CG	2.35	0.56
1:A:1304:LEU:CB	3:A:1:NLX:H203	2.34	0.56
1:L:6357:TRP:O	1:L:6360:PRO:HD2	2.05	0.56
1:I:3396:ILE:HB	1:I:3397:PRO:HD3	1.88	0.56
1:E:5447:TYR:HA	1:E:5527:LEU:O	2.05	0.56
1:H:2304:LEU:HD13	3:H:2:NLX:H162	1.87	0.56
1:C:3332:PRO:HB2	1:C:3333:GLU:OE1	2.06	0.56
1:K:5125:ALA:HB2	1:K:5133:LEU:CD1	2.36	0.56
1:L:6054:PRO:HG3	1:L:6078:LYS:HE2	1.86	0.56
1:J:4223:GLY:O	1:J:4226:SER:HB2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4311:ASP:HB3	1:D:4314:GLU:HG3	1.86	0.56
1:D:4057:LYS:HB3	1:D:4069:GLN:HB2	1.88	0.56
1:C:3237:LYS:HE2	1:C:3238:ASN:HD21	1.70	0.56
1:C:3359:ILE:HG23	3:C:3:NLX:H101	1.87	0.56
1:G:1104:ARG:HB3	1:G:1104:ARG:NH1	2.21	0.56
1:I:3462:LYS:HZ3	1:J:4376:LYS:HZ3	1.51	0.56
1:C:3234:PRO:O	1:C:3237:LYS:HG2	2.05	0.56
1:C:3532:ASN:HB3	1:C:3534:GLN:HE21	1.71	0.56
1:A:1236:ALA:HA	1:A:1239:LEU:HD12	1.87	0.56
1:J:4107:ASN:HD22	1:J:4108:ILE:H	1.53	0.56
1:A:1456:SER:HB3	1:A:1460:LYS:HD3	1.87	0.56
1:B:2218:PHE:CB	1:B:2244:ILE:HB	2.35	0.56
1:I:3353:GLN:O	1:I:3467:ASP:HA	2.05	0.56
1:C:3350:ILE:O	1:C:3448:GLU:HA	2.06	0.56
1:C:3144:LEU:HD13	1:C:3177:PHE:CE1	2.41	0.56
1:G:1332:PRO:O	1:G:1336:GLN:HG2	2.05	0.56
1:K:5039:SER:HB3	1:K:5046:PRO:HG3	1.87	0.56
1:D:4101:PHE:CZ	3:D:4:NLX:H21	2.41	0.56
1:G:1145:MET:CB	1:G:1304:LEU:HD21	2.36	0.56
1:L:6220:GLU:OE2	1:L:6221:SER:HB2	2.06	0.56
1:C:3423:ASP:OD1	1:C:3540:LYS:HE3	2.06	0.56
1:B:2404:LEU:N	1:B:2404:LEU:HD23	2.21	0.56
1:L:6093:ALA:HB1	3:L:6:NLX:H192	1.87	0.56
1:K:5355:PHE:HB2	1:K:5422:ALA:HB2	1.88	0.56
1:J:4135:VAL:HB	1:J:4215:VAL:HG22	1.88	0.56
1:A:1218:PHE:CB	1:A:1244:ILE:HB	2.36	0.56
1:J:4371:GLY:O	1:J:4414:LYS:HD3	2.06	0.56
1:K:5256:VAL:O	1:K:5258:LYS:HE3	2.06	0.55
1:L:6257:LYS:HB2	1:L:6322:VAL:HG12	1.88	0.55
1:A:1027:ASP:OD2	1:A:1032:LYS:HG2	2.04	0.55
1:C:3237:LYS:HE2	1:C:3238:ASN:ND2	2.21	0.55
1:I:3369:SER:HA	1:J:4368:LEU:O	2.06	0.55
1:A:1333:GLU:O	1:A:1337:ALA:HB2	2.06	0.55
1:B:2216:THR:HG23	1:B:2242:ARG:HB2	1.88	0.55
1:G:1097:LEU:HD11	1:G:1101:PHE:CE2	2.41	0.55
1:I:3353:GLN:HE22	1:I:3465:ILE:H	1.54	0.55
1:I:3088:THR:CG2	1:I:3295:LEU:HD13	2.35	0.55
1:L:6271:THR:CG2	1:L:6297:THR:HG23	2.35	0.55
1:L:6428:VAL:O	1:L:6432:ILE:HG13	2.06	0.55
1:I:3257:LYS:HE2	1:I:3316:GLN:NE2	2.21	0.55
1:K:5122:TYR:HE2	4:K:7094:HOH:O	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2297:THR:O	1:B:2301:MET:HG2	2.06	0.55
1:L:6456:SER:HB3	1:L:6460:LYS:HD3	1.89	0.55
1:H:2318:LEU:HD12	1:H:2318:LEU:C	2.25	0.55
1:A:1363:LEU:HB3	3:A:1:NLX:H91	1.87	0.55
1:C:3434:ALA:HB2	1:C:3446:MET:HE3	1.88	0.55
1:E:5309:GLN:HG2	1:E:5310:GLY:N	2.20	0.55
1:C:3396:ILE:HB	1:C:3397:PRO:HD3	1.88	0.55
1:C:3318:LEU:HD11	3:C:3:NLX:C15	2.32	0.55
1:H:2486:SER:O	1:H:2490:ILE:HG13	2.07	0.55
1:F:6268:ILE:HG12	1:F:6301:MET:HE2	1.88	0.55
1:A:1396:ILE:HB	1:A:1397:PRO:HD3	1.89	0.55
1:B:2468:HIS:CD2	3:B:2:NLX:O3	2.60	0.55
1:K:5234:PRO:O	1:K:5237:LYS:HG2	2.06	0.55
1:J:4237:LYS:HG2	1:J:4238:ASN:ND2	2.22	0.55
1:I:3447:TYR:HB3	1:I:3517:TRP:HZ2	1.71	0.55
1:H:2423:ASP:OD2	1:H:2543:GLU:HG2	2.07	0.55
1:A:1392:ALA:O	1:A:1396:ILE:HG12	2.07	0.55
1:F:6447:TYR:HB3	1:F:6517:TRP:CZ2	2.41	0.55
1:J:4343:THR:HB	1:J:4442:ALA:HB2	1.89	0.55
1:J:4304:LEU:CG	3:J:4:NLX:H203	2.34	0.55
1:L:6142:GLY:HA2	3:L:6:NLX:C8	2.36	0.55
1:L:6099:GLU:HG3	1:L:6107:ASN:OD1	2.07	0.55
1:B:2262:LYS:O	1:B:2266:GLU:HG3	2.07	0.55
1:I:3095:GLN:HG2	1:J:4309:GLN:OE1	2.07	0.55
1:A:1221:SER:HA	1:A:1247:SER:O	2.07	0.55
1:I:3173:GLY:HA3	4:I:7644:HOH:O	2.06	0.55
1:D:4478:ALA:N	1:D:4479:PRO:CD	2.70	0.55
1:L:6144:LEU:HB3	1:L:6177:PHE:CE2	2.41	0.55
1:J:4331:THR:OG1	1:J:4334:GLU:HG3	2.07	0.55
1:I:3249:VAL:HG23	1:I:3251:LEU:H	1.72	0.55
1:G:1313:ARG:HA	1:G:1386:TYR:CD2	2.42	0.55
1:B:2130:LYS:HE3	1:B:2132:ARG:HG2	1.89	0.55
1:B:2180:THR:HG23	1:B:2185:SER:HB3	1.89	0.55
1:G:1383:TRP:CH2	1:G:1393:LYS:HB2	2.41	0.55
1:H:2024:PRO:HD3	1:H:2037:PHE:CD1	2.41	0.55
1:G:1197:ALA:O	1:G:1201:VAL:HG23	2.07	0.55
1:K:5220:GLU:HG2	1:K:5472:LEU:HD21	1.90	0.54
1:F:6371:GLY:O	1:F:6414:LYS:HG2	2.06	0.54
1:G:1392:ALA:HB3	1:G:1395:LEU:HG	1.89	0.54
1:J:4478:ALA:N	1:J:4479:PRO:CD	2.70	0.54
1:E:5437:HIS:HD2	1:E:5444:THR:OG1	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:2223:GLY:O	1:H:2227:VAL:HG23	2.07	0.54
1:H:2258:LYS:H	1:H:2258:LYS:HD2	1.70	0.54
1:C:3447:TYR:C	1:C:3447:TYR:CD2	2.79	0.54
1:B:2354:GLU:HB2	1:B:2422:ALA:HB1	1.89	0.54
1:B:2478:ALA:N	1:B:2479:PRO:CD	2.70	0.54
1:H:2222:ALA:CB	4:H:7211:HOH:O	2.55	0.54
1:D:4145:MET:HG3	1:D:4304:LEU:CD1	2.37	0.54
1:L:6524:GLU:OE2	1:L:6538:LYS:HG2	2.06	0.54
1:F:6104:ARG:O	1:F:6482:LYS:HE3	2.07	0.54
1:G:1323:ILE:HG13	1:G:1331:THR:HG22	1.89	0.54
1:D:4318:LEU:C	1:D:4318:LEU:HD12	2.28	0.54
1:I:3119:LEU:HD12	1:I:3119:LEU:O	2.06	0.54
1:D:4265:ALA:HB1	1:D:4282:MET:HE1	1.89	0.54
1:K:5022:SER:N	4:K:7180:HOH:O	2.40	0.54
1:G:1086:MET:HE2	1:G:1148:ALA:HB2	1.90	0.54
1:K:5112:LEU:N	1:K:5112:LEU:HD12	2.23	0.54
1:G:1313:ARG:HG2	1:G:1386:TYR:CE2	2.42	0.54
1:E:5313:ARG:HG2	1:E:5386:TYR:CE2	2.43	0.54
1:C:3329:LEU:HG	4:C:7056:HOH:O	2.06	0.54
1:F:6512:GLU:H	1:F:6512:GLU:CD	2.11	0.54
1:I:3491:ARG:HB3	1:I:3491:ARG:NH1	2.22	0.54
1:K:5221:SER:O	1:K:5225:GLU:N	2.37	0.54
1:L:6395:LEU:HD22	1:L:6550:LEU:CD1	2.37	0.54
1:K:5149:ALA:CB	1:K:5169:GLN:HG3	2.38	0.54
1:E:5105:LYS:HE2	1:E:5483:GLU:HG3	1.88	0.54
1:K:5505:ARG:NH1	4:K:7766:HOH:O	2.40	0.54
1:B:2237:LYS:HB2	4:B:7015:HOH:O	2.07	0.54
1:J:4420:LEU:CD1	1:J:4547:TRP:HZ2	2.21	0.54
1:I:3243:ALA:O	1:I:3346:TYR:HA	2.07	0.54
1:K:5079:ASN:ND2	2:K:579:NAG:C1	2.71	0.54
1:D:4244:ILE:HG12	1:D:4347:MET:HB3	1.90	0.54
1:H:2363:LEU:CD1	3:H:2:NLX:H101	2.36	0.54
1:D:4215:VAL:H	1:D:4241:HIS:CD2	2.07	0.54
1:L:6105:LYS:CD	1:L:6106:GLU:HG3	2.37	0.54
1:A:1333:GLU:CD	1:A:1333:GLU:H	2.11	0.54
1:F:6540:LYS:HA	1:F:6543:GLU:OE1	2.08	0.54
1:E:5333:GLU:OE1	1:E:5333:GLU:N	2.33	0.54
1:C:3089:GLN:OE1	1:C:3146:VAL:HB	2.07	0.54
1:I:3278:THR:OG1	1:I:3281:VAL:HG23	2.07	0.54
1:D:4124:PRO:HD3	1:D:4158:ALA:HB1	1.89	0.54
1:G:1304:LEU:CD1	1:G:1318:LEU:HB3	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:2316:GLN:OE1	1:H:2317:PRO:HD2	2.07	0.54
1:I:3420:LEU:HD13	1:I:3547:TRP:CZ2	2.43	0.54
1:F:6257:LYS:HB2	1:F:6322:VAL:HG12	1.90	0.54
1:H:2420:LEU:HD12	1:H:2547:TRP:HZ2	1.73	0.54
1:I:3218:PHE:HB3	1:I:3244:ILE:HB	1.90	0.54
1:F:6264:LEU:O	1:F:6264:LEU:HD22	2.07	0.54
1:J:4456:SER:HB3	1:J:4460:LYS:HD3	1.90	0.54
1:A:1134:PRO:CG	1:A:1163:VAL:HG12	2.32	0.53
1:A:1079:ASN:HD22	2:A:179:NAG:H2	1.74	0.53
1:K:5394:GLU:HG3	1:K:5395:LEU:HG	1.91	0.53
1:C:3404:LEU:O	1:C:3406:GLY:N	2.41	0.53
1:A:1131:ASN:O	1:A:1132:ARG:HG2	2.07	0.53
1:L:6177:PHE:HB2	1:L:6319:LEU:HD22	1.90	0.53
1:A:1318:LEU:O	1:A:1318:LEU:HD12	2.08	0.53
1:I:3428:VAL:O	1:I:3432:ILE:HG13	2.08	0.53
1:C:3404:LEU:C	1:C:3406:GLY:H	2.11	0.53
1:H:2456:SER:HB2	1:H:2460:LYS:CD	2.39	0.53
1:G:1092:LYS:HZ1	1:L:6302:LYS:HB2	1.73	0.53
1:D:4386:TYR:N	1:D:4387:PRO:HD2	2.23	0.53
1:D:4091:PRO:HB3	1:D:4112:LEU:HD11	1.90	0.53
1:J:4264:LEU:CD1	1:J:4316:GLN:HG2	2.38	0.53
1:E:5252:THR:HG22	1:E:5252:THR:O	2.08	0.53
1:L:6358:LEU:HG	1:L:6363:LEU:CD1	2.38	0.53
1:K:5357:TRP:O	1:K:5361:MET:HB2	2.08	0.53
1:C:3370:GLU:HG3	1:D:4461:PRO:CG	2.39	0.53
1:G:1435:ARG:HH12	1:G:1544:VAL:HG11	1.73	0.53
1:D:4132:ARG:HB3	1:D:4211:ASN:HB2	1.91	0.53
1:H:2540:LYS:O	1:H:2544:VAL:HG23	2.09	0.53
1:H:2216:THR:HG23	1:H:2242:ARG:HB2	1.90	0.53
1:L:6359:ILE:HD11	1:L:6468:HIS:ND1	2.23	0.53
1:I:3217:ILE:CD1	1:I:3227:VAL:HG13	2.38	0.53
1:H:2104:ARG:HG2	1:H:2104:ARG:HH11	1.73	0.53
1:G:1132:ARG:HB3	1:G:1211:ASN:HB2	1.89	0.53
1:F:6271:THR:HG22	1:F:6297:THR:HG23	1.90	0.53
1:A:1260:ASP:OD2	1:A:1263:PRO:HD3	2.08	0.53
1:G:1026:VAL:CG1	1:G:1027:ASP:N	2.71	0.53
1:E:5480:PHE:HZ	1:E:5494:LYS:HG2	1.72	0.53
1:G:1303:PHE:HB2	4:G:7512:HOH:O	2.07	0.53
1:E:5126:ASP:H	1:E:5131:ASN:ND2	2.07	0.53
1:E:5355:PHE:HD1	1:E:5418:LEU:HD22	1.73	0.53
1:L:6130:LYS:H	1:L:6130:LYS:HE3	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2112:LEU:O	1:B:2113:SER:HB2	2.07	0.53
1:I:3462:LYS:HZ3	1:J:4376:LYS:NZ	2.05	0.53
1:D:4251:LEU:CD2	1:D:4333:GLU:HG3	2.39	0.53
1:D:4131:ASN:O	1:D:4132:ARG:NH1	2.42	0.53
1:A:1392:ALA:HB1	1:A:1394:GLU:OE2	2.08	0.53
1:I:3343:THR:HG22	1:I:3442:ALA:HB2	1.91	0.53
1:L:6251:LEU:CD2	1:L:6333:GLU:HG3	2.38	0.53
1:F:6537:GLN:O	1:F:6538:LYS:HB2	2.08	0.53
1:B:2318:LEU:HG	3:B:2:N LX:C17	2.36	0.53
1:B:2083:TYR:CZ	1:B:2108:ILE:HD13	2.43	0.53
1:D:4353:GLN:O	1:D:4467:ASP:HA	2.09	0.53
1:B:2095:GLN:O	1:B:2099:GLU:HG3	2.08	0.53
1:A:1539:LEU:HG	1:A:1540:LYS:HG2	1.89	0.53
1:G:1552:ALA:O	1:G:1553:LYS:HB2	2.07	0.53
1:A:1289:LYS:HA	1:A:1293:GLU:OE2	2.08	0.53
1:F:6097:LEU:HB2	3:F:6:N LX:C19	2.39	0.53
1:G:1404:LEU:HB3	1:G:1413:LYS:CG	2.39	0.53
1:L:6324:ASP:OD1	1:L:6326:MET:N	2.39	0.53
1:B:2452:ARG:HD2	1:B:2464:VAL:O	2.08	0.53
1:E:5098:SER:O	1:E:5102:THR:HB	2.09	0.53
1:B:2043:PHE:HB3	4:B:7515:HOH:O	2.08	0.53
1:F:6026:VAL:CG1	1:F:6207:SER:HB3	2.39	0.53
1:H:2355:PHE:CE1	1:H:2360:PRO:HB3	2.43	0.53
1:G:1349:GLY:HA3	1:G:1447:TYR:CE1	2.43	0.53
1:C:3364:MET:CE	3:C:3:N LX:C18	2.73	0.53
1:I:3357:TRP:O	1:I:3360:PRO:HD2	2.09	0.53
1:A:1086:MET:CE	1:A:1110:LEU:HB2	2.39	0.53
1:J:4313:ARG:HD3	1:J:4383:TRP:HH2	1.74	0.53
1:I:3348:VAL:O	1:I:3446:MET:HA	2.08	0.53
1:L:6417:PHE:O	1:L:6420:LEU:HB3	2.08	0.53
1:C:3302:LYS:HD2	1:D:4092:LYS:HD3	1.90	0.53
1:L:6235:LEU:HD12	1:L:6327:LEU:CD1	2.32	0.53
1:G:1304:LEU:HD11	1:G:1318:LEU:HD23	1.89	0.53
1:I:3355:PHE:CE1	1:I:3360:PRO:HG3	2.44	0.53
1:I:3429:PRO:O	1:I:3433:VAL:HG23	2.08	0.53
1:H:2306:LEU:HD22	1:H:2366:TYR:CE1	2.44	0.53
1:G:1086:MET:HE3	1:G:1110:LEU:HD12	1.90	0.53
1:C:3382:LEU:HD11	1:C:3420:LEU:HD11	1.90	0.53
3:H:2:N LX:H203	3:H:2:N LX:O4	2.09	0.52
3:D:4:N LX:O2	4:D:7001:HOH:O	2.19	0.52
1:F:6359:ILE:HA	3:F:6:N LX:H162	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:4132:ARG:HH12	1:J:4206:ALA:HB2	1.73	0.52
1:E:5308:LEU:HD21	1:E:5367:PRO:HG2	1.90	0.52
1:B:2149:ALA:CB	1:B:2169:GLN:HG3	2.39	0.52
1:G:1026:VAL:HG12	1:G:1027:ASP:N	2.24	0.52
1:E:5140:HIS:CD2	1:E:5147:GLY:HA3	2.44	0.52
1:K:5342:HIS:HA	4:K:7948:HOH:O	2.08	0.52
1:H:2350:ILE:HD12	1:H:2350:ILE:O	2.09	0.52
1:H:2107:ASN:ND2	1:H:2108:ILE:H	2.07	0.52
1:E:5313:ARG:HA	1:E:5386:TYR:CD2	2.45	0.52
1:H:2024:PRO:HD3	1:H:2037:PHE:CE1	2.45	0.52
1:D:4266:GLU:O	1:D:4270:ILE:HG13	2.08	0.52
1:C:3092:LYS:CD	1:D:4302:LYS:HD2	2.39	0.52
1:I:3250:ALA:O	1:I:3256:VAL:HG21	2.08	0.52
1:H:2097:LEU:HD11	1:H:2101:PHE:CE2	2.45	0.52
1:K:5465:ILE:N	1:K:5465:ILE:HD12	2.24	0.52
1:G:1218:PHE:HB2	1:G:1244:ILE:HB	1.91	0.52
1:I:3386:TYR:O	1:I:3390:CYS:N	2.40	0.52
1:B:2103:ASN:ND2	1:B:2481:LEU:HD12	2.24	0.52
1:H:2260:ASP:OD1	1:H:2263:PRO:HD3	2.10	0.52
1:L:6023:PRO:HB2	1:L:6034:LEU:CD2	2.38	0.52
1:F:6258:LYS:CE	1:F:6258:LYS:H	2.21	0.52
1:K:5370:GLU:O	1:K:5372:GLN:HG3	2.10	0.52
1:G:1348:VAL:O	1:G:1446:MET:HA	2.10	0.52
1:C:3286:LEU:HA	1:C:3289:LYS:HG2	1.92	0.52
1:A:1278:THR:HG21	1:C:3115:ASP:OD2	2.10	0.52
1:C:3024:PRO:HG3	1:C:3037:PHE:CZ	2.45	0.52
1:E:5348:VAL:O	1:E:5446:MET:HA	2.09	0.52
1:H:2370:GLU:C	1:H:2372:GLN:N	2.63	0.52
1:G:1221:SER:HB2	3:G:1:NLX:O1	2.10	0.52
1:G:1452:ARG:HG2	1:G:1452:ARG:NH1	2.24	0.52
1:K:5246:GLU:O	1:K:5247:SER:HB2	2.10	0.52
1:L:6533:THR:O	1:L:6534:GLN:HG3	2.10	0.52
1:E:5140:HIS:HD2	1:E:5141:GLY:O	1.92	0.52
1:D:4089:GLN:OE1	1:D:4146:VAL:HB	2.10	0.52
1:L:6526:TYR:HE1	1:L:6528:GLN:HG2	1.74	0.52
1:H:2228:SER:CB	1:H:2250:ALA:H	2.23	0.52
1:E:5404:LEU:CD2	1:E:5416:LEU:HB2	2.40	0.52
1:L:6290:THR:OG1	1:L:6293:GLU:HG3	2.09	0.52
1:I:3432:ILE:O	1:I:3435:ARG:HB2	2.09	0.52
1:L:6225:GLU:HG3	1:L:6255:LEU:HD13	1.91	0.52
1:J:4482:LYS:HE2	4:J:7544:HOH:O	2.07	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:5538:LYS:O	1:E:5541:ASP:HB2	2.08	0.52
1:I:3152:TYR:CD1	1:I:3152:TYR:N	2.77	0.52
1:I:3026:VAL:HG12	1:I:3027:ASP:N	2.24	0.52
1:K:5223:GLY:O	1:K:5227:VAL:HG23	2.10	0.52
1:F:6097:LEU:HD13	3:F:6:N LX:C19	2.40	0.52
1:A:1133:LEU:HB3	1:A:1134:PRO:HD2	1.91	0.52
1:I:3215:VAL:H	1:I:3241:HIS:CD2	2.25	0.52
1:F:6395:LEU:HD13	1:F:6550:LEU:HD23	1.91	0.52
1:K:5428:VAL:O	1:K:5432:ILE:HG13	2.09	0.52
1:B:2396:ILE:HB	1:B:2397:PRO:HD3	1.91	0.52
1:C:3436:ASN:N	1:C:3436:ASN:HD22	2.08	0.52
1:K:5367:PRO:C	1:K:5368:LEU:HD12	2.30	0.52
1:H:2371:GLY:HA2	1:H:2414:LYS:CD	2.37	0.52
1:J:4431:VAL:HG21	1:J:4540:LYS:HB2	1.92	0.52
1:J:4079:ASN:ND2	2:J:479:NAG:C5	2.72	0.52
1:K:5186:ARG:HB3	1:K:5324:ASP:HB2	1.91	0.52
1:E:5297:THR:O	1:E:5301:MET:HG2	2.10	0.52
1:K:5346:TYR:HB3	1:K:5437:HIS:CD2	2.45	0.52
1:A:1498:LYS:CD	1:A:1514:LEU:HD11	2.30	0.52
1:I:3490:ILE:O	1:I:3494:LYS:HG3	2.10	0.52
1:A:1351:ASN:ND2	1:A:1449:PHE:HB3	2.25	0.52
1:J:4104:ARG:NH2	1:J:4150:SER:O	2.40	0.52
1:B:2340:ASN:HB3	4:B:7205:HOH:O	2.08	0.52
1:J:4100:LEU:O	1:J:4101:PHE:HD1	1.93	0.52
1:I:3389:VAL:HB	1:I:3424:VAL:HG11	1.92	0.52
1:J:4252:THR:O	1:J:4254:VAL:N	2.43	0.52
1:D:4235:LEU:HD12	1:D:4327:LEU:HD12	1.90	0.52
1:K:5392:ALA:O	1:K:5396:ILE:HG12	2.09	0.52
1:I:3407:THR:HG21	1:I:3412:LYS:HD3	1.92	0.52
1:G:1399:ALA:HB2	1:G:1550:LEU:CD2	2.40	0.52
1:F:6529:ILE:HA	1:F:6533:THR:HG23	1.91	0.52
1:G:1233:SER:OG	1:G:1327:LEU:HD12	2.10	0.52
1:B:2190:GLY:O	1:B:2194:GLN:HG3	2.09	0.52
1:D:4042:GLY:N	4:D:7218:HOH:O	2.43	0.52
1:B:2452:ARG:HG2	1:B:2452:ARG:HH11	1.75	0.51
1:D:4023:PRO:HB2	1:D:4034:LEU:HD21	1.90	0.51
1:I:3330:LYS:HG3	1:I:3335:LEU:HD21	1.92	0.51
1:H:2459:MET:SD	1:K:5308:LEU:HD22	2.50	0.51
1:H:2079:ASN:OD1	2:H:279:NAG:C1	2.58	0.51
1:H:2409:ASP:OD2	1:H:2412:LYS:HB2	2.10	0.51
1:F:6359:ILE:HG12	3:F:6:N LX:H151	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2359:ILE:HG23	3:B:2:NLX:C7	2.40	0.51
1:I:3364:MET:HE1	3:I:3:NLX:H171	1.92	0.51
1:E:5370:GLU:C	1:E:5372:GLN:H	2.13	0.51
1:C:3186:ARG:HB3	1:C:3324:ASP:HB2	1.91	0.51
1:F:6107:ASN:HD22	1:F:6108:ILE:N	2.07	0.51
1:G:1371:GLY:C	1:G:1414:LYS:HD3	2.30	0.51
1:I:3151:THR:HB	1:I:3152:TYR:CD1	2.44	0.51
1:K:5278:THR:OG1	1:K:5281:VAL:HG23	2.10	0.51
1:E:5079:ASN:HD21	2:E:579:NAG:C1	2.22	0.51
1:A:1402:LYS:O	1:A:1402:LYS:HG3	2.10	0.51
1:B:2359:ILE:HD13	3:B:2:NLX:H72	1.91	0.51
1:E:5363:LEU:HD13	3:E:5:NLX:H203	1.91	0.51
1:L:6304:LEU:CD2	3:L:6:NLX:H102	2.38	0.51
1:L:6188:ASN:ND2	1:L:6327:LEU:HD23	2.25	0.51
1:C:3371:GLY:O	1:C:3411:VAL:HG13	2.10	0.51
1:E:5491:ARG:HG2	1:E:5491:ARG:HH11	1.74	0.51
1:D:4420:LEU:HD12	1:D:4420:LEU:C	2.31	0.51
1:J:4230:LEU:O	1:J:4342:HIS:HE1	1.93	0.51
1:L:6410:THR:HA	1:L:6413:LYS:HG3	1.91	0.51
1:C:3104:ARG:O	1:C:3482:LYS:HE3	2.09	0.51
1:K:5057:LYS:HG3	1:K:5058:PRO:HD2	1.92	0.51
1:H:2501:ALA:O	1:H:2505:ARG:HG2	2.09	0.51
1:J:4221:SER:OG	3:J:4:NLX:O1	2.28	0.51
1:G:1145:MET:HE1	1:G:1303:PHE:HD1	1.76	0.51
1:B:2527:LEU:HD11	1:B:2533:THR:HG22	1.93	0.51
1:I:3386:TYR:N	1:I:3387:PRO:HD2	2.25	0.51
1:E:5220:GLU:HG3	4:E:7086:HOH:O	2.11	0.51
1:K:5110:LEU:HD11	1:K:5150:SER:HB2	1.92	0.51
1:A:1215:VAL:N	1:A:1241:HIS:HD2	1.96	0.51
1:H:2343:THR:HB	1:H:2442:ALA:HB2	1.92	0.51
1:A:1462:LYS:HE3	1:F:6374:ASP:OD2	2.10	0.51
1:C:3100:LEU:HD13	1:C:3358:LEU:CD1	2.41	0.51
1:F:6426:PHE:O	1:F:6429:PRO:HD2	2.10	0.51
1:E:5203:ASP:OD1	1:E:5203:ASP:N	2.42	0.51
1:J:4174:ILE:HA	1:J:4319:LEU:HD12	1.92	0.51
1:A:1304:LEU:CG	3:A:1:NLX:H203	2.40	0.51
1:F:6214:SER:HA	1:F:6241:HIS:CD2	2.45	0.51
1:J:4313:ARG:HA	1:J:4386:TYR:CD2	2.45	0.51
1:G:1339:ARG:NH1	1:G:1436:ASN:HD22	2.09	0.51
1:I:3431:VAL:HG21	1:I:3540:LYS:HB2	1.93	0.51
1:D:4427:GLY:O	1:D:4431:VAL:HG23	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:4542:LYS:HB2	4:J:7954:HOH:O	2.09	0.51
1:G:1120:ASN:HB2	1:G:1167:THR:OG1	2.11	0.51
1:A:1124:PRO:HD3	1:A:1158:ALA:HB1	1.92	0.51
1:K:5063:LEU:O	1:K:5066:THR:HG23	2.11	0.51
1:J:4235:LEU:HD12	1:J:4327:LEU:HD12	1.92	0.51
1:I:3139:ILE:HG12	1:I:3168:ILE:HD11	1.91	0.51
1:E:5354:GLU:HA	1:E:5354:GLU:OE1	2.11	0.51
1:E:5318:LEU:HD11	3:E:5:NLX:H11	1.92	0.51
1:A:1104:ARG:HG2	1:A:1104:ARG:HH11	1.74	0.51
1:C:3333:GLU:N	1:C:3333:GLU:OE1	2.43	0.51
1:K:5217:ILE:CD1	1:K:5227:VAL:HG13	2.41	0.51
1:D:4289:LYS:HA	1:D:4293:GLU:OE2	2.11	0.51
1:E:5107:ASN:HD22	1:E:5108:ILE:N	2.08	0.51
1:B:2493:SER:O	1:B:2497:MET:HG3	2.11	0.51
1:F:6025:VAL:HG22	1:F:6034:LEU:HD23	1.92	0.51
1:E:5126:ASP:H	1:E:5131:ASN:HD21	1.56	0.51
1:I:3029:VAL:HG23	1:I:3204:ASN:OD1	2.11	0.51
1:E:5478:ALA:N	1:E:5479:PRO:CD	2.74	0.51
1:I:3364:MET:SD	3:I:3:NLX:H201	2.50	0.51
1:H:2176:GLY:CA	1:H:2189:TRP:HB2	2.38	0.51
1:A:1435:ARG:O	1:A:1438:ARG:HB3	2.11	0.51
1:H:2104:ARG:HG2	1:H:2104:ARG:NH1	2.26	0.51
1:B:2531:ALA:C	1:B:2532:ASN:HD22	2.13	0.51
1:G:1334:GLU:O	1:G:1338:GLU:HG2	2.11	0.51
1:B:2179:SER:O	1:B:2265:ALA:HB2	2.11	0.51
1:L:6444:THR:HG22	1:L:6520:TYR:HB3	1.92	0.51
1:I:3400:THR:HG23	1:I:3404:LEU:HD12	1.92	0.51
1:I:3236:ALA:O	1:I:3239:LEU:HB2	2.11	0.51
1:H:2252:THR:HG22	1:H:2252:THR:O	2.11	0.51
1:K:5371:GLY:CA	1:K:5414:LYS:HD3	2.37	0.51
1:A:1364:MET:HG3	3:A:1:NLX:H82	1.92	0.51
1:H:2268:ILE:HD11	1:H:2319:LEU:HD21	1.91	0.51
1:E:5034:LEU:HB3	1:E:5079:ASN:HA	1.92	0.51
1:E:5220:GLU:HA	1:E:5246:GLU:O	2.11	0.51
1:I:3338:GLU:HB2	1:I:3340:ASN:HB2	1.93	0.51
1:G:1350:ILE:C	1:G:1351:ASN:HD22	2.14	0.51
1:H:2492:LEU:O	1:H:2496:VAL:HG23	2.11	0.51
1:A:1486:SER:O	1:A:1490:ILE:HG13	2.11	0.51
1:K:5393:LYS:HA	1:K:5396:ILE:CG1	2.41	0.50
1:A:1431:VAL:HG11	1:A:1544:VAL:HG21	1.92	0.50
1:K:5429:PRO:O	1:K:5433:VAL:HG23	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1355:PHE:CE2	1:G:1425:MET:HE2	2.46	0.50
1:B:2385:SER:C	1:B:2387:PRO:HD2	2.32	0.50
1:I:3244:ILE:HG23	1:I:3347:MET:HB3	1.92	0.50
1:E:5220:GLU:HG2	1:E:5472:LEU:HD21	1.92	0.50
1:A:1045:GLN:HB2	1:L:6486:SER:HA	1.93	0.50
1:G:1526:TYR:CD2	1:G:1539:LEU:HB2	2.45	0.50
1:J:4508:ASN:OD1	1:J:4510:ASN:HB2	2.11	0.50
1:H:2097:LEU:HD11	3:H:2:N LX:H11	1.93	0.50
1:K:5420:LEU:HD12	1:K:5547:TRP:CZ2	2.44	0.50
1:L:6420:LEU:HD13	1:L:6547:TRP:CZ2	2.46	0.50
1:F:6447:TYR:CD2	1:F:6447:TYR:C	2.85	0.50
1:D:4171:ARG:O	1:D:4176:GLY:HA3	2.11	0.50
1:L:6452:ARG:HD2	1:L:6464:VAL:O	2.11	0.50
1:G:1152:TYR:CD1	1:G:1152:TYR:N	2.79	0.50
1:C:3143:GLY:CA	3:C:3:N LX:H152	2.34	0.50
1:B:2359:ILE:CG1	3:B:2:N LX:C7	2.85	0.50
1:J:4363:LEU:HD22	3:J:4:N LX:H192	1.93	0.50
1:J:4332:PRO:O	1:J:4336:GLN:HG2	2.11	0.50
1:I:3467:ASP:OD1	1:I:3468:HIS:N	2.41	0.50
1:J:4262:LYS:HB3	1:J:4263:PRO:HD3	1.92	0.50
1:I:3125:ALA:HB1	1:I:3131:ASN:ND2	2.25	0.50
1:L:6386:TYR:N	1:L:6387:PRO:HD2	2.27	0.50
1:D:4197:ALA:O	1:D:4201:VAL:HG23	2.11	0.50
1:G:1105:LYS:HE3	1:G:1483:GLU:OE1	2.12	0.50
1:J:4532:ASN:HB2	4:J:7463:HOH:O	2.10	0.50
1:C:3143:GLY:HA2	3:C:3:N LX:H51	1.94	0.50
1:D:4101:PHE:CE2	3:D:4:N LX:H21	2.46	0.50
1:D:4447:TYR:CD2	1:D:4447:TYR:C	2.84	0.50
1:L:6225:GLU:HG3	1:L:6255:LEU:CD1	2.42	0.50
1:I:3223:GLY:O	1:I:3227:VAL:HG23	2.10	0.50
1:E:5372:GLN:HB3	4:E:7425:HOH:O	2.11	0.50
1:I:3526:TYR:CD2	1:I:3539:LEU:HB2	2.46	0.50
1:G:1234:PRO:O	1:G:1237:LYS:HB2	2.12	0.50
1:H:2283:VAL:O	1:H:2287:ARG:HB2	2.11	0.50
1:A:1498:LYS:HD3	1:A:1502:ASN:HD21	1.76	0.50
1:J:4363:LEU:HD22	3:J:4:N LX:H181	1.92	0.50
1:K:5363:LEU:HB3	3:K:5:N LX:H201	1.93	0.50
1:G:1244:ILE:HD11	1:G:1503:PHE:HD2	1.76	0.50
1:K:5524:GLU:O	1:K:5537:GLN:O	2.29	0.50
1:K:5517:TRP:CE3	1:K:5527:LEU:HD23	2.47	0.50
1:E:5527:LEU:HD11	1:E:5533:THR:HG22	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:3404:LEU:HD22	1:I:3413:LYS:O	2.10	0.50
1:I:3252:THR:HG23	1:I:3425:MET:O	2.12	0.50
1:D:4121:ILE:HG12	1:D:4166:VAL:HG22	1.94	0.50
1:F:6161:GLU:HG3	1:F:6501:ALA:HB2	1.93	0.50
1:D:4543:GLU:OE2	1:D:4543:GLU:N	2.31	0.50
1:E:5412:LYS:O	1:E:5416:LEU:HG	2.11	0.50
1:F:6543:GLU:H	1:F:6543:GLU:CD	2.14	0.50
1:F:6428:VAL:HG21	1:F:6547:TRP:CD1	2.47	0.50
1:I:3330:LYS:HG3	1:I:3335:LEU:CD2	2.41	0.50
1:E:5079:ASN:ND2	2:E:579:NAG:C1	2.75	0.50
1:C:3104:ARG:CZ	1:C:3153:ASP:HB2	2.41	0.50
1:L:6149:ALA:HB2	1:L:6169:GLN:HG3	1.94	0.50
1:I:3103:ASN:ND2	1:I:3481:LEU:HD12	2.25	0.50
1:H:2144:LEU:HD22	1:H:2177:PHE:CZ	2.46	0.50
3:K:5:N LX:O4	3:K:5:N LX:H203	2.12	0.50
1:J:4452:ARG:HD2	1:J:4464:VAL:O	2.12	0.50
1:L:6420:LEU:C	1:L:6420:LEU:HD12	2.32	0.50
1:I:3218:PHE:HA	1:I:3244:ILE:O	2.12	0.50
1:K:5370:GLU:C	1:K:5372:GLN:H	2.15	0.50
1:I:3038:VAL:HG12	1:I:3039:SER:N	2.26	0.50
1:G:1363:LEU:HD22	3:G:1:N LX:H181	1.94	0.50
1:H:2257:LYS:CE	1:H:2316:GLN:HE22	2.25	0.50
1:K:5264:LEU:HD21	1:K:5319:LEU:HD23	1.94	0.50
1:D:4480:PHE:O	1:D:4481:LEU:HD23	2.12	0.50
1:A:1463:THR:HG21	1:F:6372:GLN:CB	2.41	0.50
1:J:4526:TYR:CE1	1:J:4539:LEU:HD13	2.46	0.50
1:F:6252:THR:HG22	1:F:6254:VAL:HG12	1.93	0.50
1:F:6242:ARG:HD3	1:F:6503:PHE:O	2.12	0.50
1:D:4126:ASP:OD2	1:D:4129:LYS:HG3	2.12	0.50
1:I:3257:LYS:NZ	1:I:3316:GLN:CG	2.75	0.50
1:G:1383:TRP:CZ3	1:G:1393:LYS:HB2	2.47	0.50
1:I:3309:GLN:HG3	1:J:4095:GLN:NE2	2.27	0.50
1:K:5271:THR:HG22	1:K:5297:THR:HG23	1.94	0.50
1:G:1260:ASP:O	1:G:1263:PRO:HD2	2.12	0.50
1:E:5158:ALA:O	1:E:5162:ASN:HA	2.11	0.50
1:I:3134:PRO:HG2	1:I:3163:VAL:HG12	1.94	0.50
1:L:6143:GLY:HA3	3:L:6:N LX:H11	1.94	0.49
1:G:1304:LEU:HD13	1:G:1318:LEU:HB3	1.93	0.49
1:H:2420:LEU:HD12	1:H:2547:TRP:CZ2	2.46	0.49
1:F:6186:ARG:HB3	1:F:6324:ASP:HB2	1.94	0.49
1:L:6260:ASP:O	1:L:6263:PRO:HD2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:6545:ALA:HA	1:L:6548:THR:HG22	1.93	0.49
1:J:4074:TRP:CD2	1:J:4078:LYS:HE2	2.47	0.49
1:L:6086:MET:HE2	1:L:6110:LEU:HB2	1.93	0.49
1:L:6086:MET:HE3	1:L:6110:LEU:HB2	1.93	0.49
1:J:4370:GLU:HB3	1:J:4372:GLN:HG2	1.93	0.49
1:K:5268:ILE:HD11	1:K:5319:LEU:HD21	1.94	0.49
1:D:4201:VAL:HG13	1:D:4205:ILE:HB	1.94	0.49
1:B:2053:ILE:HD12	1:B:2121:ILE:HD12	1.94	0.49
1:A:1233:SER:OG	1:A:1327:LEU:HD12	2.12	0.49
1:E:5135:VAL:HG21	1:E:5205:ILE:HG21	1.93	0.49
1:K:5540:LYS:O	1:K:5544:VAL:HG23	2.13	0.49
1:B:2024:PRO:O	1:B:2034:LEU:HD23	2.12	0.49
1:L:6420:LEU:HD11	1:L:6547:TRP:CZ2	2.46	0.49
1:I:3079:ASN:OD1	2:I:379:NAG:C1	2.60	0.49
1:A:1348:VAL:O	1:A:1446:MET:HA	2.11	0.49
1:A:1145:MET:HB2	1:A:1304:LEU:CD2	2.42	0.49
1:D:4161:GLU:OE2	1:D:4498:LYS:CA	2.60	0.49
1:E:5370:GLU:O	1:E:5372:GLN:N	2.45	0.49
1:G:1283:VAL:O	1:G:1287:ARG:HG3	2.12	0.49
1:L:6317:PRO:HG3	1:L:6387:PRO:HB2	1.94	0.49
1:I:3275:LYS:HG3	4:I:7145:HOH:O	2.11	0.49
1:A:1297:THR:O	1:A:1301:MET:HG2	2.12	0.49
1:J:4119:LEU:O	1:J:4119:LEU:HD12	2.12	0.49
1:E:5143:GLY:O	1:E:5318:LEU:HD22	2.13	0.49
1:G:1420:LEU:O	1:G:1424:VAL:HG23	2.12	0.49
1:K:5351:ASN:ND2	1:K:5449:PHE:HB3	2.27	0.49
1:I:3218:PHE:CB	1:I:3244:ILE:HB	2.43	0.49
1:C:3070:PRO:HG2	4:C:7964:HOH:O	2.12	0.49
1:L:6138:TRP:HA	1:L:6218:PHE:O	2.12	0.49
1:A:1382:LEU:HD22	1:A:1420:LEU:HD21	1.93	0.49
1:A:1105:LYS:HD2	1:A:1483:GLU:OE2	2.12	0.49
1:C:3304:LEU:HD22	3:C:3:N LX:H201	1.95	0.49
1:H:2359:ILE:CD1	3:H:2:N LX:H71	2.39	0.49
1:K:5258:LYS:H	1:K:5258:LYS:CD	2.06	0.49
1:L:6304:LEU:HD13	3:L:6:N LX:C18	2.41	0.49
1:K:5304:LEU:HD13	3:K:5:N LX:C18	2.37	0.49
1:F:6414:LYS:HD2	1:F:6414:LYS:C	2.32	0.49
1:K:5311:ASP:OD1	1:K:5313:ARG:HB2	2.12	0.49
1:J:4414:LYS:O	1:J:4418:LEU:HG	2.12	0.49
1:B:2478:ALA:HB3	1:B:2479:PRO:HD3	1.93	0.49
1:C:3092:LYS:HZ3	1:D:4302:LYS:HD2	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:6471:GLU:O	1:L:6475:VAL:HG23	2.12	0.49
1:A:1302:LYS:HG3	4:A:7839:HOH:O	2.12	0.49
1:F:6090:ASP:HB3	1:F:6093:ALA:HB3	1.93	0.49
1:B:2355:PHE:CD2	1:B:2359:ILE:HG21	2.48	0.49
1:J:4359:ILE:HG23	3:J:4:NLX:C8	2.43	0.49
1:D:4447:TYR:HA	1:D:4527:LEU:O	2.13	0.49
1:E:5491:ARG:CD	4:E:7007:HOH:O	2.61	0.49
1:C:3313:ARG:HG2	1:C:3386:TYR:CZ	2.48	0.49
1:H:2264:LEU:HD21	1:H:2319:LEU:HD23	1.95	0.49
1:L:6198:LEU:HD21	1:L:6217:ILE:CG2	2.42	0.49
1:A:1350:ILE:O	1:A:1448:GLU:HA	2.12	0.49
1:H:2103:ASN:ND2	1:H:2481:LEU:HD12	2.28	0.49
1:J:4244:ILE:HG12	1:J:4347:MET:HB3	1.94	0.49
1:H:2057:LYS:HD2	4:H:7830:HOH:O	2.12	0.49
1:H:2304:LEU:HD22	3:H:2:NLX:C20	2.42	0.49
1:G:1468:HIS:NE2	3:G:1:NLX:O1	2.46	0.49
1:K:5393:LYS:HA	1:K:5396:ILE:HG12	1.93	0.49
1:J:4525:GLY:CA	1:J:4537:GLN:HG2	2.42	0.49
1:I:3229:VAL:HG11	1:I:3327:LEU:HD21	1.94	0.49
1:D:4335:LEU:HD11	4:D:7303:HOH:O	2.12	0.49
1:K:5428:VAL:HG13	1:K:5544:VAL:HG22	1.94	0.49
1:H:2348:VAL:O	1:H:2446:MET:HA	2.12	0.49
1:J:4473:PHE:HA	4:J:7950:HOH:O	2.11	0.49
1:K:5060:LEU:CD2	1:K:5114:GLU:HB2	2.43	0.49
1:H:2374:ASP:O	1:H:2376:LYS:N	2.46	0.49
1:I:3025:VAL:HG22	1:I:3034:LEU:HD23	1.94	0.49
1:C:3308:LEU:HG	4:C:7642:HOH:O	2.11	0.49
1:A:1023:PRO:HB2	1:A:1034:LEU:HD21	1.95	0.49
1:B:2359:ILE:HB	1:B:2360:PRO:HD3	1.91	0.49
1:H:2404:LEU:HD13	1:H:2413:LYS:CG	2.43	0.49
1:A:1375:GLN:O	1:A:1378:ALA:HB3	2.12	0.49
1:I:3355:PHE:CD1	1:I:3360:PRO:HG3	2.48	0.49
1:C:3540:LYS:O	1:C:3544:VAL:HG23	2.13	0.49
1:I:3330:LYS:HB3	1:I:3330:LYS:NZ	2.27	0.49
1:H:2349:GLY:HA3	1:H:2447:TYR:CE1	2.48	0.49
1:G:1149:ALA:HB2	1:G:1168:ILE:O	2.12	0.49
1:F:6375:GLN:HG3	1:F:6400:THR:HG22	1.94	0.49
1:D:4024:PRO:HD3	1:D:4037:PHE:CD1	2.48	0.49
1:G:1374:ASP:O	1:G:1376:LYS:N	2.46	0.49
1:G:1079:ASN:ND2	2:G:179:NAG:C1	2.76	0.49
1:E:5404:LEU:HD22	1:E:5416:LEU:HB2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:5468:HIS:NE2	3:K:5:N LX:O3	2.46	0.49
1:A:1304:LEU:HG	3:A:1:N LX:H151	1.93	0.49
1:B:2452:ARG:NH1	4:B:7528:HOH:O	2.44	0.49
1:F:6478:ALA:N	1:F:6479:PRO:CD	2.75	0.49
1:J:4182:ASP:HB2	1:J:4183:GLU:OE2	2.13	0.49
1:J:4297:THR:O	1:J:4301:MET:HG2	2.13	0.49
1:E:5068:PRO:HB3	1:E:5193:ASP:OD1	2.13	0.49
1:H:2402:LYS:HG2	1:H:2546:PHE:CE1	2.47	0.49
1:G:1216:THR:OG1	1:G:1504:ALA:HA	2.12	0.49
1:L:6051:LEU:HD13	1:L:6083:TYR:CD1	2.48	0.49
1:D:4034:LEU:HD12	1:D:4079:ASN:OD1	2.13	0.49
1:L:6264:LEU:O	1:L:6268:ILE:HD13	2.12	0.49
1:J:4176:GLY:HA2	1:J:4189:TRP:HB2	1.95	0.49
1:K:5101:PHE:CE1	1:K:5469:GLY:HA3	2.48	0.49
1:B:2251:LEU:HB2	1:B:2429:PRO:HB3	1.95	0.49
1:G:1523:LYS:HB3	1:G:1537:GLN:OE1	2.12	0.49
1:G:1292:GLU:HG2	4:G:7529:HOH:O	2.11	0.49
1:H:2204:ASN:O	1:H:2206:ALA:N	2.45	0.49
1:I:3543:GLU:OE2	1:I:3543:GLU:N	2.41	0.49
1:L:6304:LEU:HB3	3:L:6:N LX:H172	1.94	0.48
1:K:5361:MET:SD	1:K:5363:LEU:HG	2.52	0.48
1:G:1104:ARG:HH12	1:G:1153:ASP:HB2	1.78	0.48
1:C:3024:PRO:HG3	1:C:3037:PHE:CE1	2.47	0.48
1:G:1338:GLU:O	1:G:1340:ASN:N	2.46	0.48
1:E:5339:ARG:HG2	1:E:5339:ARG:NH1	2.28	0.48
1:J:4278:THR:OG1	1:J:4281:VAL:HG23	2.13	0.48
1:A:1330:LYS:HB2	1:A:1335:LEU:CD2	2.43	0.48
1:E:5024:PRO:HD3	1:E:5037:PHE:CD1	2.47	0.48
1:C:3464:VAL:HG22	1:D:4370:GLU:OE1	2.13	0.48
1:A:1269:ALA:HB2	1:A:1282:MET:HE3	1.94	0.48
1:C:3156:ALA:O	1:C:3160:HIS:HB2	2.13	0.48
1:K:5359:ILE:HG12	3:K:5:N LX:H151	1.96	0.48
1:B:2079:ASN:HD21	2:B:279:NAG:C1	2.26	0.48
1:B:2370:GLU:O	1:B:2372:GLN:HG3	2.13	0.48
1:E:5452:ARG:HE	1:E:5462:LYS:HA	1.78	0.48
1:D:4309:GLN:NE2	1:D:4310:GLY:N	2.61	0.48
1:B:2308:LEU:HD22	1:E:5459:MET:SD	2.53	0.48
1:G:1142:GLY:CA	3:G:1:N LX:H152	2.43	0.48
1:C:3257:LYS:HE3	1:C:3322:VAL:HG12	1.95	0.48
1:K:5215:VAL:H	1:K:5241:HIS:CD2	2.19	0.48
1:K:5420:LEU:CD1	1:K:5547:TRP:HZ2	2.24	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:5538:LYS:HB3	1:E:5541:ASP:HB2	1.95	0.48
1:E:5176:GLY:HA2	1:E:5189:TRP:HB2	1.95	0.48
1:J:4187:GLY:O	1:J:4188:ASN:HB2	2.13	0.48
1:K:5380:SER:O	1:K:5384:LYS:HG2	2.13	0.48
1:J:4551:PHE:C	1:J:4553:LYS:H	2.16	0.48
1:B:2254:VAL:HG21	1:B:2388:LEU:HD23	1.95	0.48
1:F:6202:GLN:NE2	1:F:6212:PRO:O	2.46	0.48
1:H:2237:LYS:O	1:H:2238:ASN:HB2	2.11	0.48
1:A:1304:LEU:HG	3:A:1:NLX:O4	2.12	0.48
1:L:6478:ALA:N	1:L:6479:PRO:CD	2.76	0.48
1:A:1068:PRO:HA	4:A:7198:HOH:O	2.13	0.48
1:B:2255:LEU:HD23	1:B:2318:LEU:HD13	1.94	0.48
1:K:5353:GLN:O	1:K:5467:ASP:HA	2.13	0.48
1:G:1318:LEU:O	1:G:1318:LEU:HD12	2.12	0.48
1:C:3112:LEU:O	1:C:3113:SER:HB2	2.13	0.48
1:A:1358:LEU:O	1:A:1363:LEU:HD12	2.14	0.48
1:I:3251:LEU:HD12	1:I:3433:VAL:CG2	2.44	0.48
1:I:3251:LEU:HD21	1:I:3333:GLU:HG3	1.96	0.48
1:E:5338:GLU:O	1:E:5338:GLU:HG3	2.13	0.48
1:K:5478:ALA:N	1:K:5479:PRO:CD	2.76	0.48
1:G:1087:CYS:O	1:G:1088:THR:C	2.51	0.48
1:A:1251:LEU:HD12	1:A:1433:VAL:CG2	2.43	0.48
1:F:6145:MET:HE1	1:F:6303:PHE:CD1	2.48	0.48
1:J:4145:MET:HG3	1:J:4304:LEU:HD11	1.96	0.48
1:G:1304:LEU:CG	3:G:1:NLX:H203	2.36	0.48
1:C:3268:ILE:HG12	1:C:3301:MET:CE	2.44	0.48
1:F:6188:ASN:ND2	1:F:6324:ASP:OD2	2.44	0.48
1:A:1311:ASP:OD1	1:A:1313:ARG:HB2	2.14	0.48
1:C:3290:THR:HG23	1:C:3293:GLU:OE2	2.12	0.48
1:G:1308:LEU:HD22	1:L:6459:MET:SD	2.53	0.48
1:F:6136:MET:HB3	1:F:6218:PHE:HE1	1.79	0.48
1:K:5349:GLY:HA3	1:K:5447:TYR:CE1	2.49	0.48
1:G:1086:MET:HE1	4:G:7232:HOH:O	2.13	0.48
1:B:2520:TYR:CZ	1:B:2524:GLU:HG2	2.49	0.48
1:H:2297:THR:O	1:H:2301:MET:HG2	2.14	0.48
1:H:2101:PHE:CE2	3:H:2:NLX:H21	2.49	0.48
1:G:1140:HIS:CD2	1:G:1147:GLY:HA3	2.48	0.48
1:J:4079:ASN:CG	2:J:479:NAG:C1	2.82	0.48
1:E:5286:LEU:HA	1:E:5289:LYS:HG3	1.96	0.48
1:B:2292:GLU:O	1:B:2296:GLU:HG3	2.13	0.48
1:L:6182:ASP:HB2	1:L:6183:GLU:OE2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2143:GLY:O	1:B:2144:LEU:HB2	2.14	0.48
1:L:6324:ASP:OD1	1:L:6327:LEU:N	2.36	0.48
1:I:3426:PHE:HE2	3:I:3:NLX:HO11	1.60	0.48
1:K:5217:ILE:O	1:K:5243:ALA:HA	2.14	0.48
1:L:6492:LEU:O	1:L:6496:VAL:HG23	2.14	0.48
1:K:5099:GLU:HG3	1:K:5107:ASN:OD1	2.13	0.48
1:C:3026:VAL:HG13	4:C:7260:HOH:O	2.13	0.48
1:A:1284:HIS:O	1:A:1288:GLN:OE1	2.32	0.48
1:A:1024:PRO:HD3	1:A:1037:PHE:CD1	2.48	0.48
1:D:4140:HIS:HD2	1:D:4141:GLY:O	1.97	0.48
1:H:2363:LEU:HD22	3:H:2:NLX:H181	1.94	0.48
1:H:2143:GLY:HA3	3:H:2:NLX:C15	2.44	0.48
1:D:4143:GLY:O	1:D:4145:MET:HG2	2.13	0.48
1:F:6359:ILE:HG12	3:F:6:NLX:C15	2.43	0.48
1:B:2318:LEU:CD1	3:B:2:NLX:H171	2.43	0.48
1:B:2174:ILE:CG1	1:B:2298:THR:HG22	2.44	0.48
1:I:3324:ASP:OD2	1:I:3327:LEU:HB3	2.13	0.48
1:K:5104:ARG:HH11	1:K:5104:ARG:HG2	1.78	0.48
1:E:5465:ILE:HD12	1:E:5465:ILE:N	2.29	0.48
1:E:5215:VAL:H	1:E:5241:HIS:CD2	2.28	0.48
1:J:4079:ASN:ND2	2:J:479:NAG:H5	2.26	0.48
1:F:6107:ASN:HD22	1:F:6108:ILE:H	1.62	0.48
1:C:3475:VAL:HG22	1:C:3496:VAL:HG11	1.96	0.48
1:K:5404:LEU:O	1:K:5413:LYS:HE2	2.13	0.48
1:H:2478:ALA:N	1:H:2479:PRO:CD	2.77	0.48
1:E:5502:ASN:O	1:E:5506:ASN:HB2	2.14	0.48
1:B:2499:PHE:HZ	1:B:2515:PRO:HG2	1.78	0.48
1:E:5404:LEU:HD22	1:E:5413:LYS:O	2.14	0.48
1:J:4130:LYS:HD3	1:J:4131:ASN:N	2.27	0.48
1:K:5550:LEU:HD23	1:K:5550:LEU:C	2.34	0.48
1:D:4461:PRO:HG2	1:D:4464:VAL:CG2	2.44	0.48
1:E:5187:GLY:O	1:E:5188:ASN:HB2	2.14	0.48
1:I:3257:LYS:HZ3	1:I:3316:GLN:CG	2.27	0.48
1:C:3436:ASN:N	1:C:3436:ASN:ND2	2.61	0.48
1:A:1040:LEU:HD22	1:A:1156:ALA:HA	1.96	0.48
1:K:5309:GLN:NE2	4:K:7219:HOH:O	2.42	0.48
1:E:5039:SER:OG	1:E:5046:PRO:HG3	2.14	0.48
1:G:1478:ALA:N	1:G:1479:PRO:CD	2.77	0.48
1:H:2202:GLN:HG2	4:H:7675:HOH:O	2.13	0.48
1:J:4353:GLN:NE2	1:J:4465:ILE:H	2.12	0.48
1:H:2311:ASP:HB3	1:H:2314:GLU:HG2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3543:GLU:OE2	1:C:3543:GLU:N	2.42	0.48
1:H:2143:GLY:O	1:H:2318:LEU:HD22	2.14	0.47
1:D:4296:GLU:O	1:D:4300:LYS:HG3	2.14	0.47
1:G:1104:ARG:CZ	1:G:1153:ASP:HB2	2.43	0.47
1:B:2223:GLY:O	1:B:2227:VAL:HG23	2.14	0.47
1:D:4423:ASP:OD1	1:D:4540:LYS:CE	2.62	0.47
1:F:6140:HIS:CD2	1:F:6147:GLY:HA3	2.49	0.47
1:A:1024:PRO:HB3	1:A:1037:PHE:CZ	2.49	0.47
1:H:2338:GLU:HB3	1:H:2340:ASN:OD1	2.14	0.47
1:B:2420:LEU:C	1:B:2420:LEU:HD12	2.34	0.47
1:D:4382:LEU:HD11	1:D:4391:ILE:HD12	1.95	0.47
1:K:5100:LEU:HD22	1:K:5457:SER:HB2	1.96	0.47
1:I:3492:LEU:O	1:I:3496:VAL:HG23	2.14	0.47
1:A:1128:THR:HG23	4:A:7990:HOH:O	2.13	0.47
1:G:1161:GLU:OE2	1:G:1498:LYS:HG2	2.14	0.47
1:H:2368:LEU:HB2	1:K:5369:SER:HA	1.95	0.47
1:G:1134:PRO:CG	1:G:1163:VAL:HG12	2.29	0.47
1:J:4319:LEU:N	1:J:4319:LEU:HD23	2.28	0.47
1:I:3237:LYS:O	1:I:3238:ASN:HB2	2.14	0.47
1:H:2385:SER:O	1:H:2389:VAL:HG22	2.15	0.47
1:H:2225:GLU:O	1:H:2228:SER:N	2.47	0.47
1:L:6313:ARG:HG2	1:L:6386:TYR:CE2	2.49	0.47
1:B:2143:GLY:HA3	3:B:2:NLX:H161	1.96	0.47
1:B:2359:ILE:CB	1:B:2360:PRO:CD	2.91	0.47
1:G:1034:LEU:O	1:G:1081:THR:HG23	2.15	0.47
1:D:4257:LYS:NZ	1:D:4316:GLN:HG3	2.28	0.47
1:J:4412:LYS:O	1:J:4416:LEU:HG	2.14	0.47
1:J:4349:GLY:HA3	1:J:4447:TYR:CE1	2.50	0.47
1:J:4417:PHE:O	1:J:4420:LEU:HB3	2.14	0.47
1:H:2350:ILE:C	1:H:2350:ILE:HD12	2.35	0.47
1:J:4218:PHE:N	1:J:4218:PHE:CD1	2.82	0.47
1:F:6409:ASP:OD2	1:F:6412:LYS:HB2	2.14	0.47
1:I:3044:ALA:O	1:I:3046:PRO:HD3	2.13	0.47
1:C:3304:LEU:HD22	3:C:3:NLX:C20	2.43	0.47
1:A:1249:VAL:HB	1:A:1433:VAL:HG21	1.96	0.47
1:J:4363:LEU:CD1	3:J:4:NLX:H181	2.32	0.47
1:G:1302:LYS:HB2	1:L:6092:LYS:NZ	2.29	0.47
1:G:1417:PHE:HD1	1:G:1420:LEU:HD23	1.79	0.47
1:B:2220:GLU:OE1	1:B:2221:SER:CB	2.58	0.47
1:E:5257:LYS:HA	4:E:7588:HOH:O	2.13	0.47
1:C:3092:LYS:HD2	1:D:4302:LYS:HD2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:6396:ILE:HB	1:F:6397:PRO:HD3	1.96	0.47
1:K:5354:GLU:HB2	1:K:5422:ALA:HB1	1.96	0.47
1:I:3318:LEU:HG	3:I:3:N LX:C18	2.44	0.47
1:I:3364:MET:CG	3:I:3:N LX:H201	2.43	0.47
1:L:6414:LYS:O	1:L:6418:LEU:HG	2.14	0.47
1:K:5104:ARG:NH1	1:K:5104:ARG:HG2	2.29	0.47
1:G:1547:TRP:CZ3	1:G:1550:LEU:HD23	2.50	0.47
1:F:6107:ASN:ND2	1:F:6108:ILE:N	2.62	0.47
1:G:1349:GLY:HA3	1:G:1447:TYR:CZ	2.50	0.47
1:F:6375:GLN:HG3	1:F:6400:THR:CG2	2.45	0.47
1:J:4183:GLU:OE2	1:J:4183:GLU:N	2.47	0.47
1:A:1119:LEU:HD12	1:A:1119:LEU:O	2.15	0.47
1:H:2278:THR:OG1	1:H:2281:VAL:HG23	2.14	0.47
1:I:3024:PRO:HG3	1:I:3037:PHE:CE2	2.50	0.47
1:I:3225:GLU:CB	1:I:3255:LEU:HD13	2.44	0.47
1:K:5363:LEU:HD13	3:K:5:N LX:C20	2.45	0.47
1:A:1375:GLN:NE2	1:A:1400:THR:HG22	2.25	0.47
1:K:5549:ASN:O	1:K:5552:ALA:HB3	2.15	0.47
1:L:6447:TYR:HB3	1:L:6517:TRP:CZ2	2.50	0.47
1:I:3258:LYS:CE	1:I:3258:LYS:H	2.27	0.47
1:J:4302:LYS:HZ3	1:J:4302:LYS:HB3	1.77	0.47
1:A:1218:PHE:HB3	1:A:1244:ILE:HB	1.94	0.47
1:J:4277:THR:HG21	1:L:6113:SER:HB2	1.96	0.47
1:G:1518:PRO:HG2	4:G:7779:HOH:O	2.14	0.47
1:H:2035:GLY:HA2	1:H:2081:THR:HG22	1.97	0.47
1:E:5428:VAL:O	1:E:5429:PRO:C	2.50	0.47
1:C:3402:LYS:HG2	1:C:3546:PHE:CE1	2.49	0.47
1:J:4449:PHE:CE2	1:J:4471:GLU:HA	2.50	0.47
1:D:4145:MET:CG	1:D:4304:LEU:HD11	2.45	0.47
1:G:1241:HIS:O	1:G:1242:ARG:HD3	2.15	0.47
1:E:5363:LEU:HB3	3:E:5:N LX:C20	2.35	0.47
1:L:6145:MET:HB3	1:L:6304:LEU:HD11	1.96	0.47
1:L:6363:LEU:HD22	3:L:6:N LX:C20	2.44	0.47
1:H:2417:PHE:O	1:H:2420:LEU:HB3	2.15	0.47
1:H:2366:TYR:OH	1:H:2385:SER:HB3	2.15	0.47
1:D:4478:ALA:HB3	1:D:4479:PRO:HD3	1.96	0.47
1:G:1380:SER:O	1:G:1383:TRP:HB3	2.15	0.47
1:J:4264:LEU:HG	1:J:4316:GLN:HG2	1.96	0.47
1:L:6526:TYR:CZ	1:L:6536:ALA:HB3	2.50	0.47
1:E:5339:ARG:HG2	1:E:5339:ARG:HH11	1.80	0.47
1:J:4258:LYS:HD3	1:J:4258:LYS:N	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:5456:SER:HB3	1:E:5460:LYS:HD2	1.97	0.47
1:B:2092:LYS:HD2	1:E:5302:LYS:HE3	1.97	0.47
1:I:3301:MET:HB2	1:I:3303:PHE:CE1	2.49	0.47
1:A:1296:GLU:O	1:A:1300:LYS:HG3	2.15	0.47
1:I:3191:HIS:CD2	1:I:3321:THR:HG23	2.50	0.47
1:J:4398:GLU:OE2	1:J:4550:LEU:HD13	2.15	0.47
1:I:3366:TYR:HA	1:I:3367:PRO:HD3	1.76	0.47
1:A:1201:VAL:O	1:A:1205:ILE:HB	2.14	0.47
1:A:1304:LEU:HD12	1:A:1318:LEU:HD23	1.96	0.47
1:I:3428:VAL:HG21	1:I:3547:TRP:CD1	2.48	0.47
1:I:3478:ALA:O	1:I:3482:LYS:HB2	2.15	0.47
1:G:1262:LYS:HB3	1:G:1263:PRO:HD3	1.97	0.47
1:B:2366:TYR:HD2	1:B:2368:LEU:HD13	1.79	0.47
1:G:1508:ASN:OD1	1:G:1510:ASN:HB2	2.15	0.47
1:H:2101:PHE:HE2	3:H:2:NLX:H21	1.80	0.47
1:G:1302:LYS:CG	1:L:6092:LYS:HZ3	2.20	0.47
1:A:1374:ASP:O	1:A:1375:GLN:C	2.54	0.47
1:I:3221:SER:OG	1:I:3222:ALA:N	2.47	0.47
1:I:3125:ALA:HB2	1:I:3133:LEU:CD1	2.45	0.47
1:G:1140:HIS:HE1	4:G:7298:HOH:O	1.97	0.47
1:I:3381:LEU:CD2	1:J:4459:MET:HG2	2.44	0.47
1:G:1354:GLU:HG3	1:G:1426:PHE:HB2	1.97	0.47
1:K:5264:LEU:HD22	1:K:5316:GLN:NE2	2.29	0.47
1:J:4218:PHE:HD1	1:J:4218:PHE:N	2.12	0.47
1:I:3024:PRO:HG3	1:I:3037:PHE:CZ	2.49	0.47
1:K:5254:VAL:O	1:K:5254:VAL:HG22	2.15	0.47
1:B:2074:TRP:CD2	1:B:2078:LYS:HE2	2.50	0.47
1:C:3395:LEU:HB3	1:C:3550:LEU:HD11	1.97	0.47
1:L:6339:ARG:HH21	1:L:6439:ASP:HB2	1.80	0.47
1:H:2126:ASP:OD1	1:H:2128:THR:HG23	2.14	0.47
1:H:2363:LEU:CB	3:H:2:NLX:H181	2.25	0.47
1:A:1304:LEU:CD2	3:A:1:NLX:H151	2.45	0.47
1:L:6029:VAL:HG13	4:L:7981:HOH:O	2.15	0.47
1:G:1201:VAL:O	1:G:1205:ILE:HB	2.14	0.47
1:E:5083:TYR:CE2	1:E:5108:ILE:HD13	2.49	0.47
1:G:1087:CYS:HB3	4:G:7585:HOH:O	2.15	0.47
1:E:5114:GLU:HG3	1:E:5291:GLU:OE2	2.16	0.47
1:H:2179:SER:O	1:H:2265:ALA:HB2	2.15	0.47
1:D:4304:LEU:HB3	3:D:4:NLX:C20	2.40	0.46
1:K:5258:LYS:CD	1:K:5258:LYS:N	2.71	0.46
1:I:3317:PRO:C	3:I:3:NLX:H192	2.36	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:4376:LYS:HA	1:J:4379:MET:HE2	1.96	0.46
1:J:4107:ASN:HD22	1:J:4108:ILE:N	2.12	0.46
1:E:5437:HIS:CD2	1:E:5444:THR:OG1	2.69	0.46
1:L:6136:MET:HB3	1:L:6218:PHE:CE1	2.50	0.46
1:G:1513:GLY:O	1:G:1514:LEU:HD23	2.15	0.46
1:L:6499:PHE:HD2	1:L:6509:PRO:O	1.99	0.46
1:K:5407:THR:OG1	1:K:5408:ASP:N	2.48	0.46
1:L:6435:ARG:NH1	1:L:6544:VAL:HG11	2.30	0.46
1:K:5068:PRO:HB3	1:K:5193:ASP:OD1	2.14	0.46
1:H:2375:GLN:NE2	1:H:2400:THR:HG22	2.30	0.46
1:L:6480:PHE:CD1	1:L:6480:PHE:N	2.83	0.46
1:F:6143:GLY:O	1:F:6145:MET:HG2	2.15	0.46
3:B:2:N LX:O4	3:B:2:N LX:H203	2.15	0.46
1:K:5420:LEU:CD1	1:K:5547:TRP:CZ2	2.98	0.46
1:L:6107:ASN:HD22	1:L:6108:ILE:H	1.63	0.46
1:G:1543:GLU:O	1:G:1547:TRP:CD1	2.68	0.46
1:D:4041:GLU:HB3	4:D:7218:HOH:O	2.14	0.46
1:A:1188:ASN:O	1:A:1189:TRP:C	2.53	0.46
1:E:5183:GLU:OE2	1:E:5183:GLU:N	2.41	0.46
1:F:6142:GLY:C	3:F:6:N LX:H82	2.36	0.46
1:K:5395:LEU:HD13	1:K:5550:LEU:HD23	1.98	0.46
1:E:5540:LYS:O	1:E:5544:VAL:HG23	2.15	0.46
1:H:2359:ILE:HG12	3:H:2:N LX:C8	2.46	0.46
1:F:6330:LYS:HG3	1:F:6335:LEU:CD2	2.44	0.46
1:G:1438:ARG:NH1	1:G:1524:GLU:HG2	2.31	0.46
1:L:6416:LEU:O	1:L:6419:ASP:HB2	2.15	0.46
1:J:4318:LEU:O	1:J:4318:LEU:HD12	2.16	0.46
1:J:4274:CYS:SG	1:J:4285:CYS:SG	3.04	0.46
1:I:3368:LEU:O	1:J:4369:SER:HA	2.14	0.46
1:G:1437:HIS:O	1:G:1440:ALA:HB3	2.16	0.46
1:B:2403:TYR:O	1:B:2416:LEU:HD13	2.15	0.46
1:L:6363:LEU:HB3	3:L:6:N LX:C20	2.44	0.46
1:H:2386:TYR:N	1:H:2387:PRO:CD	2.78	0.46
1:L:6107:ASN:HD22	1:L:6108:ILE:N	2.13	0.46
1:K:5447:TYR:HB3	1:K:5517:TRP:CZ2	2.51	0.46
1:K:5264:LEU:HD22	1:K:5316:GLN:HE21	1.80	0.46
1:I:3218:PHE:N	1:I:3218:PHE:CD1	2.84	0.46
1:G:1211:ASN:HD22	1:G:1214:SER:HB3	1.80	0.46
1:F:6120:ASN:HB2	1:F:6167:THR:OG1	2.16	0.46
1:A:1129:LYS:HD3	4:A:7882:HOH:O	2.15	0.46
1:K:5183:GLU:OE2	1:K:5183:GLU:N	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1216:THR:HG23	1:G:1242:ARG:HB2	1.96	0.46
1:H:2241:HIS:C	1:H:2242:ARG:HD2	2.36	0.46
1:A:1099:GLU:HG2	1:A:1107:ASN:OD1	2.16	0.46
1:A:1220:GLU:OE2	1:A:1221:SER:HB2	2.16	0.46
1:B:2452:ARG:HG2	1:B:2452:ARG:NH1	2.29	0.46
1:I:3446:MET:HE1	1:I:3539:LEU:HD23	1.97	0.46
1:A:1394:GLU:O	1:A:1397:PRO:HD2	2.14	0.46
1:F:6492:LEU:HD12	1:F:6495:MET:HE2	1.97	0.46
1:K:5160:HIS:CE1	1:K:5480:PHE:CE2	3.04	0.46
1:H:2353:GLN:HG3	1:H:2465:ILE:O	2.16	0.46
1:I:3057:LYS:HD3	1:I:3063:LEU:HD11	1.98	0.46
1:E:5343:THR:HB	1:E:5442:ALA:HB2	1.98	0.46
1:G:1079:ASN:CG	2:G:179:NAG:C1	2.84	0.46
1:K:5550:LEU:C	1:K:5552:ALA:H	2.18	0.46
1:E:5491:ARG:NE	4:E:7007:HOH:O	2.42	0.46
1:E:5373:LEU:H	1:E:5410:THR:HB	1.81	0.46
1:B:2218:PHE:HB3	1:B:2244:ILE:HB	1.98	0.46
1:F:6268:ILE:HG12	1:F:6301:MET:CE	2.46	0.46
1:G:1086:MET:CE	1:G:1148:ALA:HB2	2.45	0.46
1:B:2428:VAL:HG13	1:B:2544:VAL:HG22	1.96	0.46
1:C:3375:GLN:HB3	1:C:3375:GLN:HE21	1.57	0.46
1:H:2361:MET:CE	1:H:2363:LEU:HG	2.46	0.46
1:H:2363:LEU:HD22	3:H:2:NLX:C18	2.46	0.46
1:F:6359:ILE:CD1	3:F:6:NLX:H151	2.45	0.46
1:B:2304:LEU:HD23	3:B:2:NLX:H191	1.98	0.46
1:E:5358:LEU:HG	1:E:5363:LEU:HD12	1.98	0.46
1:L:6060:LEU:CD2	1:L:6114:GLU:HB3	2.45	0.46
1:I:3096:LEU:HD13	1:J:4309:GLN:HB2	1.98	0.46
1:C:3329:LEU:C	1:C:3330:LYS:HG2	2.36	0.46
1:G:1536:ALA:O	1:G:1537:GLN:HG2	2.16	0.46
1:C:3140:HIS:HD2	1:C:3141:GLY:O	1.97	0.46
1:J:4375:GLN:HE21	1:J:4375:GLN:HB3	1.55	0.46
1:B:2258:LYS:O	1:B:2258:LYS:HD2	2.16	0.46
1:A:1152:TYR:N	1:A:1152:TYR:CD1	2.84	0.46
1:G:1145:MET:HG3	1:G:1304:LEU:HD21	1.98	0.46
2:A:179:NAG:O4	2:A:180:NAG:C1	2.64	0.46
1:B:2353:GLN:HE22	1:B:2465:ILE:H	1.62	0.46
1:A:1220:GLU:HA	1:A:1246:GLU:O	2.16	0.46
1:E:5242:ARG:NH1	1:E:5242:ARG:HG3	2.28	0.46
1:G:1355:PHE:CD1	1:G:1360:PRO:HG3	2.50	0.46
1:L:6161:GLU:HB3	1:L:6501:ALA:CB	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3445:TYR:CZ	1:C:3509:PRO:HD2	2.51	0.46
1:F:6349:GLY:HA3	1:F:6447:TYR:CE1	2.51	0.46
1:L:6452:ARG:HG2	1:L:6452:ARG:HH11	1.81	0.46
1:I:3103:ASN:HD22	1:I:3481:LEU:HD12	1.80	0.46
1:F:6296:GLU:O	1:F:6300:LYS:HG3	2.15	0.46
1:F:6103:ASN:ND2	1:F:6476:PHE:HB3	2.31	0.46
1:B:2458:ASP:HB2	4:E:7333:HOH:O	2.16	0.46
1:C:3501:ALA:O	1:C:3505:ARG:HG2	2.14	0.46
1:L:6205:ILE:HD12	1:L:6205:ILE:HA	1.69	0.46
1:A:1334:GLU:O	1:A:1337:ALA:HB3	2.16	0.46
1:A:1104:ARG:NH1	1:A:1153:ASP:HB2	2.29	0.46
1:D:4251:LEU:HD12	1:D:4433:VAL:HG23	1.96	0.46
1:K:5428:VAL:N	1:K:5429:PRO:CD	2.79	0.46
1:J:4256:VAL:HG12	1:J:4258:LYS:HD2	1.98	0.46
1:H:2087:CYS:HB3	4:H:7192:HOH:O	2.15	0.46
1:D:4453:PRO:HD2	1:D:4470:ASP:OD2	2.15	0.46
1:E:5186:ARG:HB3	1:E:5324:ASP:HB2	1.98	0.46
1:H:2143:GLY:O	1:H:2144:LEU:HB2	2.16	0.45
1:E:5354:GLU:O	1:E:5468:HIS:HB2	2.17	0.45
1:J:4143:GLY:N	3:J:4:NLX:H152	2.31	0.45
1:L:6304:LEU:HD13	3:L:6:NLX:C19	2.46	0.45
1:L:6187:GLY:O	1:L:6188:ASN:HB2	2.16	0.45
1:K:5395:LEU:HD23	4:K:7575:HOH:O	2.15	0.45
1:I:3462:LYS:NZ	1:J:4376:LYS:HZ2	2.14	0.45
1:A:1386:TYR:N	1:A:1387:PRO:CD	2.79	0.45
1:A:1425:MET:O	1:A:1429:PRO:HG2	2.16	0.45
1:I:3161:GLU:HB3	1:I:3501:ALA:CB	2.46	0.45
1:B:2417:PHE:O	1:B:2420:LEU:HB3	2.15	0.45
1:H:2346:TYR:HD2	1:H:2347:MET:N	2.14	0.45
1:K:5212:PRO:HG2	4:K:7443:HOH:O	2.16	0.45
1:L:6351:ASN:ND2	4:L:7041:HOH:O	2.49	0.45
1:G:1103:ASN:ND2	1:G:1476:PHE:HB3	2.31	0.45
1:E:5091:PRO:HG3	1:E:5112:LEU:CD1	2.37	0.45
1:K:5318:LEU:HD11	3:K:5:NLX:H21	1.98	0.45
1:K:5161:GLU:CD	1:K:5498:LYS:HA	2.36	0.45
1:C:3409:ASP:HB3	1:C:3412:LYS:HB3	1.98	0.45
1:L:6349:GLY:HA3	1:L:6447:TYR:CZ	2.52	0.45
1:J:4420:LEU:HD12	1:J:4547:TRP:HZ2	1.81	0.45
1:L:6244:ILE:HG12	1:L:6347:MET:HB3	1.98	0.45
1:B:2540:LYS:O	1:B:2544:VAL:HG23	2.16	0.45
1:I:3123:THR:OG1	1:I:3164:VAL:HG22	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2124:PRO:HD3	1:B:2158:ALA:HB1	1.98	0.45
1:H:2190:GLY:O	1:H:2193:ASP:HB2	2.16	0.45
1:C:3355:PHE:CE1	1:C:3421:ILE:HG21	2.50	0.45
1:K:5431:VAL:O	1:K:5435:ARG:HG3	2.16	0.45
1:K:5368:LEU:N	1:K:5368:LEU:HD12	2.31	0.45
1:D:4215:VAL:N	1:D:4241:HIS:HD2	1.97	0.45
1:J:4251:LEU:HD12	1:J:4433:VAL:CG2	2.46	0.45
1:I:3217:ILE:HD12	1:I:3227:VAL:HG13	1.99	0.45
1:B:2023:PRO:HB2	1:B:2034:LEU:HD21	1.98	0.45
1:B:2040:LEU:HD13	1:B:2155:LEU:HD11	1.97	0.45
1:C:3142:GLY:HA3	1:C:3146:VAL:O	2.16	0.45
1:A:1289:LYS:HD3	4:A:8105:HOH:O	2.16	0.45
1:H:2338:GLU:O	1:H:2339:ARG:HD3	2.17	0.45
1:J:4073:PRO:HB2	4:J:7805:HOH:O	2.16	0.45
1:D:4182:ASP:HB2	1:D:4183:GLU:OE2	2.16	0.45
1:H:2453:PRO:C	1:H:2455:PHE:H	2.18	0.45
1:J:4498:LYS:HB3	1:J:4514:LEU:HD11	1.98	0.45
1:I:3383:TRP:CZ3	1:I:3393:LYS:HB2	2.51	0.45
1:K:5409:ASP:OD2	1:K:5412:LYS:HG3	2.16	0.45
1:H:2027:ASP:CG	1:H:2032:LYS:HZ3	2.20	0.45
1:G:1179:SER:O	1:G:1265:ALA:HB2	2.16	0.45
1:J:4455:PHE:CD2	1:J:4482:LYS:HD3	2.50	0.45
1:B:2218:PHE:HB2	1:B:2244:ILE:HB	1.99	0.45
1:I:3104:ARG:CZ	1:I:3153:ASP:HB2	2.46	0.45
1:E:5252:THR:HG22	1:E:5254:VAL:HG12	1.98	0.45
1:K:5414:LYS:HB3	1:K:5414:LYS:HE2	1.80	0.45
1:A:1351:ASN:HB3	1:A:1466:GLY:O	2.16	0.45
1:A:1372:GLN:NE2	1:A:1410:THR:HG21	2.29	0.45
1:C:3220:GLU:HA	1:C:3246:GLU:O	2.16	0.45
1:C:3092:LYS:NZ	1:D:4302:LYS:HD2	2.32	0.45
1:F:6426:PHE:C	1:F:6429:PRO:HD2	2.37	0.45
1:L:6149:ALA:CB	1:L:6169:GLN:HG3	2.47	0.45
1:K:5100:LEU:CD2	1:K:5457:SER:HB2	2.47	0.45
1:K:5486:SER:O	1:K:5490:ILE:HG13	2.17	0.45
1:E:5051:LEU:O	1:E:5080:ALA:HB1	2.16	0.45
1:F:6366:TYR:HA	1:F:6367:PRO:HD3	1.81	0.45
1:K:5237:LYS:CE	1:K:5237:LYS:HA	2.31	0.45
1:J:4093:ALA:HB1	3:J:4:NLX:H191	1.98	0.45
1:B:2372:GLN:NE2	1:E:5463:THR:HG21	2.32	0.45
1:K:5386:TYR:N	1:K:5387:PRO:HD2	2.32	0.45
1:J:4023:PRO:CB	1:J:4034:LEU:HD21	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4038:VAL:CG2	1:D:4049:ILE:HD12	2.45	0.45
1:C:3420:LEU:C	1:C:3420:LEU:HD12	2.37	0.45
1:J:4089:GLN:OE1	1:J:4146:VAL:HB	2.17	0.45
1:I:3266:GLU:O	1:I:3270:ILE:HG13	2.17	0.45
1:E:5174:ILE:HA	1:E:5319:LEU:HD13	1.99	0.45
1:L:6348:VAL:O	1:L:6446:MET:HA	2.17	0.45
1:D:4234:PRO:O	1:D:4237:LYS:HB2	2.17	0.45
1:D:4221:SER:CB	3:D:4:NLX:O1	2.65	0.45
1:J:4304:LEU:CB	3:J:4:NLX:H203	2.46	0.45
1:G:1304:LEU:HD12	1:G:1318:LEU:HD23	1.96	0.45
1:I:3143:GLY:HA2	1:I:3222:ALA:HB2	1.99	0.45
1:G:1180:THR:HG22	1:G:1282:MET:HE2	1.98	0.45
1:G:1180:THR:HB	1:G:1279:SER:OG	2.17	0.45
1:H:2423:ASP:O	1:H:2428:VAL:HG23	2.15	0.45
1:G:1395:LEU:HD22	1:G:1550:LEU:CD1	2.47	0.45
1:F:6218:PHE:HB3	1:F:6244:ILE:HB	1.99	0.45
1:C:3107:ASN:ND2	1:C:3108:ILE:H	2.14	0.45
1:K:5091:PRO:HG3	1:K:5112:LEU:CD2	2.46	0.45
1:D:4049:ILE:HD11	1:D:4155:LEU:HD13	1.98	0.45
1:A:1370:GLU:HA	1:A:1370:GLU:OE2	2.16	0.45
1:H:2528:GLN:HB2	1:H:2534:GLN:HE21	1.82	0.45
1:C:3361:MET:CE	1:C:3363:LEU:HG	2.47	0.45
1:B:2260:ASP:OD1	1:B:2263:PRO:HD3	2.16	0.45
1:H:2187:GLY:O	1:H:2188:ASN:HB2	2.17	0.45
1:L:6156:ALA:HB3	4:L:8057:HOH:O	2.17	0.45
1:I:3201:VAL:HB	4:I:7603:HOH:O	2.16	0.45
1:B:2389:VAL:HB	1:B:2424:VAL:HG11	1.98	0.45
1:D:4186:ARG:HH11	1:D:4186:ARG:HG3	1.82	0.45
1:L:6500:TRP:N	1:L:6500:TRP:HE3	2.15	0.45
1:H:2143:GLY:CA	3:H:2:NLX:H152	2.46	0.45
1:L:6414:LYS:C	1:L:6414:LYS:HD2	2.37	0.45
1:G:1265:ALA:HB1	1:G:1282:MET:HE1	1.99	0.45
1:G:1524:GLU:O	1:G:1538:LYS:N	2.50	0.45
1:K:5526:TYR:CE2	1:K:5536:ALA:HB3	2.52	0.45
1:L:6501:ALA:O	1:L:6504:ALA:HB3	2.17	0.45
1:K:5026:VAL:CG1	1:K:5027:ASP:N	2.80	0.45
1:D:4105:LYS:HG3	1:D:4481:LEU:O	2.16	0.45
1:H:2311:ASP:HA	1:H:2312:PRO:HD3	1.80	0.45
1:L:6121:ILE:HG22	1:L:6122:TYR:N	2.32	0.45
1:C:3214:SER:HA	1:C:3241:HIS:CD2	2.52	0.45
1:H:2404:LEU:HD13	1:H:2413:LYS:HG2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1373:LEU:HG	1:G:1378:ALA:HB2	1.98	0.45
1:L:6235:LEU:CD1	1:L:6327:LEU:HA	2.47	0.45
1:E:5371:GLY:C	1:E:5414:LYS:HD3	2.37	0.45
1:G:1540:LYS:O	1:G:1544:VAL:HG23	2.17	0.45
1:F:6528:GLN:O	1:F:6533:THR:HG23	2.16	0.45
1:K:5125:ALA:HB1	1:K:5131:ASN:ND2	2.32	0.45
1:F:6268:ILE:HD11	1:F:6319:LEU:HD21	1.97	0.45
1:K:5057:LYS:HG3	1:K:5058:PRO:CD	2.47	0.45
1:I:3268:ILE:HG12	1:I:3301:MET:HE2	1.98	0.45
1:K:5240:PHE:N	1:K:5240:PHE:CD1	2.85	0.45
1:A:1043:PHE:CD2	1:L:6484:GLY:HA2	2.52	0.45
1:F:6049:ILE:HG12	1:F:6122:TYR:CD2	2.52	0.45
1:E:5336:GLN:HE22	1:E:5433:VAL:HA	1.82	0.45
1:G:1079:ASN:CB	2:G:179:NAG:H82	2.34	0.45
1:E:5407:THR:HG21	1:E:5412:LYS:CB	2.41	0.45
1:E:5403:TYR:O	1:E:5416:LEU:HD13	2.17	0.45
1:K:5318:LEU:HD21	3:K:5:NLX:H11	1.97	0.45
1:I:3359:ILE:HB	1:I:3360:PRO:HD3	1.98	0.45
1:K:5487:GLU:HG2	4:K:8070:HOH:O	2.17	0.45
1:K:5125:ALA:HB2	1:K:5133:LEU:HD12	1.98	0.45
1:C:3220:GLU:HG2	1:C:3472:LEU:HD21	1.98	0.45
1:L:6251:LEU:HD21	1:L:6333:GLU:HG3	1.98	0.45
1:L:6526:TYR:CE2	1:L:6539:LEU:HA	2.51	0.45
1:I:3057:LYS:HD3	1:I:3063:LEU:CD1	2.46	0.45
1:L:6286:LEU:O	1:L:6289:LYS:HB2	2.16	0.45
1:F:6283:VAL:O	1:F:6287:ARG:HG3	2.16	0.45
1:G:1467:ASP:HB3	1:G:1470:ASP:OD1	2.17	0.45
1:A:1034:LEU:C	1:A:1034:LEU:HD13	2.38	0.44
1:E:5142:GLY:HA2	3:E:5:NLX:C8	2.42	0.44
1:E:5143:GLY:O	1:E:5144:LEU:HB2	2.16	0.44
1:J:4174:ILE:HG12	1:J:4319:LEU:HD11	1.99	0.44
1:A:1375:GLN:HE21	1:A:1375:GLN:CA	2.29	0.44
1:F:6214:SER:HA	1:F:6241:HIS:HD2	1.82	0.44
1:I:3364:MET:CE	3:I:3:NLX:H201	2.47	0.44
1:E:5257:LYS:HB2	1:E:5322:VAL:HG12	1.99	0.44
1:D:4260:ASP:OD1	1:D:4262:LYS:CB	2.65	0.44
1:K:5249:VAL:CB	1:K:5433:VAL:HG21	2.46	0.44
1:J:4493:SER:O	1:J:4497:MET:HG3	2.16	0.44
1:G:1090:ASP:HB3	1:G:1093:ALA:HB3	1.97	0.44
1:D:4437:HIS:NE2	1:D:4442:ALA:HB3	2.32	0.44
1:E:5254:VAL:HG22	1:E:5318:LEU:HD12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:4303:PHE:CB	1:J:4304:LEU:HD22	2.47	0.44
1:K:5461:PRO:HG2	1:K:5464:VAL:HG23	1.99	0.44
1:F:6452:ARG:CB	1:F:6465:ILE:HG12	2.44	0.44
1:G:1399:ALA:HB2	1:G:1550:LEU:HD21	1.98	0.44
1:B:2216:THR:HG23	1:B:2242:ARG:HB3	1.97	0.44
1:L:6161:GLU:HG3	1:L:6497:MET:O	2.18	0.44
1:G:1313:ARG:HG3	1:G:1313:ARG:NH1	2.32	0.44
1:I:3136:MET:HB3	1:I:3218:PHE:CE1	2.52	0.44
1:J:4116:CYS:O	1:J:4118:TYR:N	2.51	0.44
1:F:6227:VAL:O	1:F:6231:VAL:HG23	2.17	0.44
1:F:6236:ALA:HA	1:F:6239:LEU:HD12	1.99	0.44
1:A:1199:ARG:HG3	4:A:7447:HOH:O	2.17	0.44
1:J:4045:GLN:NE2	1:J:4046:PRO:HD2	2.32	0.44
1:D:4225:GLU:O	1:D:4229:VAL:HG23	2.17	0.44
1:I:3491:ARG:HH11	1:I:3491:ARG:HB3	1.81	0.44
1:A:1375:GLN:HG2	1:A:1413:LYS:NZ	2.32	0.44
3:I:3:NLX:O4	3:I:3:NLX:H203	2.17	0.44
1:I:3462:LYS:HZ1	1:J:4376:LYS:HZ2	1.64	0.44
1:I:3495:MET:O	1:I:3498:LYS:HB2	2.18	0.44
1:C:3361:MET:HE3	1:C:3363:LEU:HG	2.00	0.44
1:G:1049:ILE:HG12	1:G:1122:TYR:CD2	2.52	0.44
1:L:6194:GLN:OE1	1:L:6226:SER:HB3	2.18	0.44
1:C:3353:GLN:NE2	1:C:3465:ILE:H	2.15	0.44
1:H:2191:HIS:O	1:H:2195:VAL:HG23	2.18	0.44
1:F:6317:PRO:HD3	1:F:6387:PRO:HB2	1.98	0.44
1:A:1480:PHE:HZ	1:A:1494:LYS:HG3	1.83	0.44
1:B:2355:PHE:CE2	1:B:2359:ILE:CG2	2.99	0.44
1:I:3160:HIS:HE1	1:I:3480:PHE:CE2	2.36	0.44
1:J:4220:GLU:O	1:J:4221:SER:HB3	2.18	0.44
1:A:1241:HIS:O	1:A:1344:VAL:HB	2.17	0.44
1:A:1304:LEU:HG	3:A:1:NLX:H203	2.00	0.44
1:B:2023:PRO:HA	1:B:2024:PRO:HD3	1.87	0.44
1:K:5246:GLU:HG2	1:K:5447:TYR:OH	2.17	0.44
1:G:1101:PHE:CD1	1:G:1472:LEU:HD12	2.52	0.44
1:F:6501:ALA:O	1:F:6504:ALA:HB3	2.17	0.44
1:C:3361:MET:SD	1:C:3361:MET:C	2.96	0.44
1:J:4045:GLN:HE21	1:J:4046:PRO:HD2	1.81	0.44
1:L:6125:ALA:HB2	1:L:6133:LEU:HD12	1.97	0.44
1:H:2404:LEU:N	1:H:2404:LEU:HD23	2.32	0.44
1:K:5354:GLU:O	1:K:5468:HIS:HB2	2.18	0.44
1:G:1221:SER:O	1:G:1224:GLY:N	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:3143:GLY:O	1:I:3318:LEU:HD22	2.17	0.44
1:J:4251:LEU:HD12	1:J:4433:VAL:HG22	1.99	0.44
1:A:1319:LEU:H	1:A:1319:LEU:CD1	2.28	0.44
1:G:1265:ALA:HB1	1:G:1282:MET:CE	2.48	0.44
1:E:5241:HIS:HB3	4:E:7347:HOH:O	2.17	0.44
1:F:6147:GLY:HA2	4:F:7265:HOH:O	2.17	0.44
1:A:1136:MET:HB3	1:A:1218:PHE:CE1	2.53	0.44
1:I:3257:LYS:HZ3	1:I:3316:GLN:HG2	1.83	0.44
1:I:3026:VAL:HG23	1:I:3050:PHE:CZ	2.53	0.44
1:C:3262:LYS:HB3	1:C:3263:PRO:HD3	1.98	0.44
1:L:6126:ASP:O	1:L:6128:THR:N	2.51	0.44
1:B:2437:HIS:HD2	1:B:2444:THR:OG1	2.00	0.44
1:G:1267:GLN:HA	4:G:7984:HOH:O	2.18	0.44
1:L:6530:GLY:O	1:L:6531:ALA:C	2.56	0.44
1:B:2355:PHE:CD2	1:B:2359:ILE:HD12	2.53	0.44
1:J:4364:MET:HG3	3:J:4:N LX:H82	1.98	0.44
1:A:1064:ARG:O	1:A:1066:THR:HG23	2.18	0.44
1:L:6220:GLU:HG2	1:L:6472:LEU:HD21	1.99	0.44
1:G:1205:ILE:HD12	1:G:1205:ILE:HA	1.78	0.44
1:G:1191:HIS:HB2	1:G:1327:LEU:HD22	1.99	0.44
1:J:4218:PHE:HB3	1:J:4244:ILE:HB	2.00	0.44
1:J:4256:VAL:HG12	1:J:4258:LYS:CD	2.48	0.44
1:J:4072:GLU:HG2	4:K:7791:HOH:O	2.17	0.44
1:H:2064:ARG:NH1	1:H:2294:LEU:HD11	2.33	0.44
1:L:6032:LYS:HB2	1:L:6077:VAL:HG22	2.00	0.44
1:B:2455:PHE:CD2	1:B:2482:LYS:HD3	2.53	0.44
1:L:6185:SER:HB2	1:L:6283:VAL:CG2	2.48	0.44
1:G:1302:LYS:HB2	1:L:6092:LYS:HZ1	1.83	0.44
1:D:4132:ARG:HD2	4:D:7062:HOH:O	2.17	0.44
1:E:5179:SER:HB3	1:E:5187:GLY:HA3	1.98	0.44
1:G:1543:GLU:O	1:G:1547:TRP:HD1	2.00	0.44
1:K:5098:SER:O	1:K:5102:THR:HB	2.17	0.44
1:D:4258:LYS:HB2	4:D:7713:HOH:O	2.17	0.44
1:B:2285:CYS:HB2	4:B:7947:HOH:O	2.17	0.44
1:H:2351:ASN:N	1:H:2351:ASN:HD22	2.16	0.44
1:F:6097:LEU:CB	3:F:6:N LX:H192	2.47	0.44
1:H:2524:GLU:O	1:H:2537:GLN:HA	2.18	0.44
1:K:5527:LEU:HD12	1:K:5528:GLN:H	1.83	0.44
1:K:5339:ARG:HB2	1:K:5440:ALA:HA	1.99	0.44
1:K:5039:SER:HB3	1:K:5046:PRO:CB	2.48	0.44
1:I:3257:LYS:HB2	1:I:3322:VAL:HG12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:5099:GLU:O	1:E:5102:THR:HG22	2.17	0.44
1:I:3228:SER:CB	1:I:3250:ALA:H	2.31	0.44
1:B:2428:VAL:O	1:B:2432:ILE:HG13	2.18	0.44
1:B:2549:ASN:O	1:B:2550:LEU:C	2.56	0.44
1:E:5211:ASN:HD22	1:E:5214:SER:HB3	1.82	0.44
1:I:3140:HIS:CD2	1:I:3147:GLY:HA3	2.53	0.44
1:H:2132:ARG:NH1	4:H:7324:HOH:O	2.50	0.44
1:K:5235:LEU:HD12	1:K:5327:LEU:CD1	2.40	0.44
1:G:1386:TYR:N	1:G:1387:PRO:HD2	2.33	0.44
1:D:4309:GLN:HE21	1:D:4309:GLN:C	2.20	0.44
1:A:1463:THR:HG21	1:F:6372:GLN:HB3	2.00	0.44
1:B:2453:PRO:C	1:B:2455:PHE:H	2.22	0.44
1:A:1405:GLY:O	1:A:1406:GLY:C	2.56	0.44
1:I:3344:VAL:HG22	4:I:7956:HOH:O	2.16	0.44
1:B:2161:GLU:HG3	1:B:2501:ALA:HB2	1.98	0.44
1:J:4236:ALA:O	1:J:4239:LEU:HB2	2.18	0.44
1:F:6363:LEU:CD1	3:F:6:NLX:H171	2.40	0.43
1:D:4242:ARG:CG	1:D:4242:ARG:HH11	2.20	0.43
1:I:3217:ILE:HG13	1:I:3227:VAL:HG13	1.99	0.43
1:B:2294:LEU:O	1:B:2298:THR:HG23	2.18	0.43
1:G:1073:PRO:O	1:H:2186:ARG:NH2	2.51	0.43
1:C:3351:ASN:ND2	4:C:7038:HOH:O	2.51	0.43
1:I:3461:PRO:HB2	1:I:3464:VAL:HG23	2.00	0.43
1:A:1032:LYS:HD2	1:A:1077:VAL:HG22	2.00	0.43
1:F:6512:GLU:N	1:F:6512:GLU:CD	2.71	0.43
1:G:1237:LYS:O	1:G:1238:ASN:HB2	2.17	0.43
1:C:3160:HIS:NE2	1:C:3480:PHE:CD2	2.86	0.43
1:C:3260:ASP:OD1	1:C:3263:PRO:HD3	2.19	0.43
1:H:2132:ARG:HD2	4:H:7324:HOH:O	2.17	0.43
1:L:6487:GLU:HB3	4:L:7856:HOH:O	2.17	0.43
1:I:3271:THR:HG22	1:I:3297:THR:HG23	2.00	0.43
1:C:3389:VAL:HB	1:C:3424:VAL:HG11	2.00	0.43
1:D:4064:ARG:HD3	1:D:4065:PHE:CE2	2.53	0.43
1:E:5361:MET:SD	1:E:5361:MET:C	2.97	0.43
1:B:2183:GLU:OE2	1:B:2183:GLU:N	2.45	0.43
1:H:2143:GLY:N	3:H:2:NLX:H152	2.32	0.43
1:F:6097:LEU:HD12	1:F:6097:LEU:O	2.18	0.43
1:F:6386:TYR:N	1:F:6387:PRO:HD2	2.32	0.43
1:I:3480:PHE:HZ	1:I:3494:LYS:HG2	1.82	0.43
1:L:6093:ALA:HB1	3:L:6:NLX:C19	2.47	0.43
1:K:5225:GLU:OE1	1:K:5225:GLU:C	2.56	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4538:LYS:HB3	1:D:4541:ASP:HB2	1.99	0.43
1:H:2420:LEU:CD1	1:H:2547:TRP:CZ2	3.01	0.43
1:B:2051:LEU:HD13	1:B:2083:TYR:CE1	2.53	0.43
1:C:3132:ARG:HD3	1:C:3132:ARG:HA	1.78	0.43
1:J:4104:ARG:O	1:J:4482:LYS:NZ	2.51	0.43
1:I:3391:ILE:O	1:I:3392:ALA:C	2.57	0.43
1:H:2409:ASP:OD2	1:H:2412:LYS:HD2	2.18	0.43
1:B:2258:LYS:H	1:B:2258:LYS:HD2	1.83	0.43
1:I:3199:ARG:NH2	4:I:7409:HOH:O	2.47	0.43
1:B:2491:ARG:O	1:B:2492:LEU:C	2.55	0.43
1:B:2447:TYR:CD2	1:B:2447:TYR:C	2.91	0.43
1:E:5304:LEU:CD1	3:E:5:NLX:H181	2.34	0.43
1:G:1359:ILE:HG23	3:G:1:NLX:H81	1.98	0.43
1:C:3343:THR:CB	1:C:3442:ALA:HB2	2.40	0.43
1:A:1363:LEU:CB	3:A:1:NLX:H91	2.48	0.43
1:I:3143:GLY:O	1:I:3144:LEU:HB2	2.18	0.43
1:H:2176:GLY:O	1:H:2189:TRP:HB2	2.18	0.43
1:K:5449:PHE:CE2	1:K:5451:TYR:HB3	2.52	0.43
1:K:5388:LEU:HD22	1:K:5425:MET:CE	2.48	0.43
1:J:4370:GLU:O	1:J:4372:GLN:HG2	2.18	0.43
1:K:5370:GLU:C	1:K:5372:GLN:N	2.72	0.43
1:K:5217:ILE:HD12	1:K:5227:VAL:HG13	2.00	0.43
1:I:3191:HIS:O	1:I:3195:VAL:HG23	2.18	0.43
1:D:4551:PHE:C	1:D:4553:LYS:H	2.22	0.43
1:C:3200:TRP:O	1:C:3204:ASN:ND2	2.45	0.43
1:H:2106:GLU:HA	4:H:7831:HOH:O	2.19	0.43
1:B:2105:LYS:HE3	1:B:2483:GLU:OE1	2.19	0.43
1:C:3264:LEU:CD1	1:C:3316:GLN:HG2	2.47	0.43
1:G:1130:LYS:HB3	1:G:1130:LYS:HE2	1.78	0.43
1:L:6143:GLY:O	1:L:6145:MET:HG2	2.18	0.43
1:G:1403:TYR:CE2	1:G:1420:LEU:HA	2.52	0.43
1:D:4079:ASN:HB2	2:D:479:NAG:C8	2.48	0.43
1:H:2264:LEU:HD21	1:H:2319:LEU:CD2	2.47	0.43
1:A:1064:ARG:NH2	1:A:1114:GLU:OE2	2.49	0.43
1:J:4526:TYR:CZ	1:J:4539:LEU:HD13	2.52	0.43
1:G:1138:TRP:O	1:G:1168:ILE:HG12	2.18	0.43
1:B:2408:ASP:HA	1:B:2413:LYS:HE2	2.00	0.43
1:A:1508:ASN:OD1	1:A:1510:ASN:HB2	2.18	0.43
1:G:1266:GLU:O	1:G:1270:ILE:HG13	2.17	0.43
1:B:2471:GLU:O	1:B:2475:VAL:HG23	2.19	0.43
1:C:3034:LEU:HB3	1:C:3079:ASN:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:2361:MET:HG2	1:K:5367:PRO:HB3	2.00	0.43
1:B:2359:ILE:CD1	3:B:2:N LX:H72	2.48	0.43
1:B:2051:LEU:HD13	1:B:2083:TYR:CD1	2.54	0.43
1:E:5237:LYS:NZ	1:E:5340:ASN:ND2	2.67	0.43
1:L:6349:GLY:HA3	1:L:6447:TYR:CE2	2.53	0.43
1:L:6091:PRO:HB3	1:L:6112:LEU:HD11	1.99	0.43
1:C:3431:VAL:HG21	1:C:3539:LEU:O	2.18	0.43
1:E:5023:PRO:HB2	1:E:5034:LEU:HD21	2.00	0.43
1:D:4420:LEU:C	1:D:4420:LEU:CD1	2.87	0.43
1:G:1352:LYS:HD3	1:G:1450:GLN:NE2	2.33	0.43
1:I:3262:LYS:HB3	1:I:3263:PRO:HD3	1.99	0.43
1:L:6067:PRO:HG2	4:L:7322:HOH:O	2.18	0.43
1:H:2145:MET:HG3	1:H:2304:LEU:HD21	2.00	0.43
1:G:1220:GLU:O	1:G:1221:SER:HB3	2.19	0.43
1:B:2220:GLU:OE1	1:B:2221:SER:N	2.52	0.43
1:L:6336:GLN:HE22	1:L:6433:VAL:HA	1.83	0.43
1:G:1438:ARG:HH12	1:G:1524:GLU:HG2	1.83	0.43
1:G:1140:HIS:CE1	1:G:1170:TYR:CE1	3.07	0.43
1:K:5527:LEU:HG	1:K:5529:ILE:CG1	2.49	0.43
1:G:1374:ASP:O	1:G:1375:GLN:C	2.56	0.43
1:J:4239:LEU:HD23	1:J:4239:LEU:HA	1.73	0.43
1:B:2332:PRO:O	1:B:2336:GLN:HG3	2.18	0.43
1:I:3350:ILE:C	1:I:3351:ASN:HD22	2.22	0.43
1:E:5153:ASP:OD2	1:E:5155:LEU:HB2	2.19	0.43
1:E:5047:VAL:HG21	1:E:5155:LEU:HD23	2.00	0.43
1:J:4233:SER:HA	1:J:4234:PRO:HD3	1.89	0.43
1:D:4236:ALA:HA	1:D:4239:LEU:HD12	2.01	0.43
1:L:6366:TYR:HA	1:L:6367:PRO:HD3	1.75	0.43
1:D:4252:THR:HG22	1:D:4252:THR:O	2.18	0.43
1:I:3155:LEU:O	1:I:3155:LEU:HD23	2.19	0.43
1:E:5468:HIS:NE2	3:E:5:N LX:O3	2.51	0.43
1:I:3317:PRO:HB3	4:I:7891:HOH:O	2.17	0.43
1:I:3352:LYS:HE3	1:I:3450:GLN:CD	2.38	0.43
1:I:3354:GLU:O	1:I:3468:HIS:HB2	2.17	0.43
1:B:2414:LYS:HE2	1:B:2414:LYS:HB3	1.86	0.43
1:B:2139:ILE:O	1:B:2223:GLY:HA3	2.19	0.43
1:G:1252:THR:HG23	1:G:1425:MET:O	2.18	0.43
1:B:2402:LYS:HG2	1:B:2546:PHE:CZ	2.54	0.43
1:J:4140:HIS:HD2	1:J:4147:GLY:HA3	1.83	0.43
1:L:6064:ARG:NH1	1:L:6286:LEU:O	2.52	0.43
1:C:3025:VAL:HG22	1:C:3034:LEU:HD23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3435:ARG:NH2	4:C:7404:HOH:O	2.40	0.43
1:J:4185:SER:HB2	1:J:4283:VAL:HG21	2.00	0.43
1:I:3090:ASP:HB3	1:I:3093:ALA:HB3	1.98	0.43
1:B:2536:ALA:O	1:B:2537:GLN:HG3	2.18	0.43
1:L:6237:LYS:HG3	1:L:6238:ASN:ND2	2.34	0.43
1:H:2138:TRP:CZ3	1:H:2219:GLY:HA2	2.53	0.43
1:K:5087:CYS:O	1:K:5088:THR:C	2.57	0.43
1:C:3318:LEU:HD11	3:C:3:NLX:C16	2.48	0.43
1:B:2355:PHE:HA	1:B:2359:ILE:HD12	2.01	0.43
1:L:6363:LEU:HD22	3:L:6:NLX:H201	2.01	0.43
1:G:1396:ILE:HB	1:G:1397:PRO:CD	2.38	0.43
1:G:1304:LEU:HD13	1:G:1317:PRO:O	2.19	0.43
1:J:4452:ARG:HH11	1:J:4452:ARG:HG2	1.83	0.43
1:A:1361:MET:HE1	1:A:1363:LEU:HD21	2.01	0.43
1:I:3318:LEU:HD11	3:I:3:NLX:H101	2.01	0.43
1:F:6324:ASP:OD2	1:F:6327:LEU:HB3	2.19	0.43
1:A:1412:LYS:O	1:A:1416:LEU:HB2	2.19	0.43
1:G:1252:THR:HG22	1:G:1254:VAL:HG12	2.01	0.43
1:G:1384:LYS:O	1:G:1387:PRO:HD2	2.19	0.43
1:J:4353:GLN:HE22	1:J:4465:ILE:H	1.67	0.43
1:A:1445:TYR:OH	1:A:1508:ASN:ND2	2.51	0.43
1:G:1528:GLN:HB2	1:G:1534:GLN:NE2	2.34	0.43
1:C:3331:THR:OG1	1:C:3334:GLU:HG3	2.19	0.43
1:C:3414:LYS:HG3	1:C:3415:ASP:N	2.33	0.43
1:H:2303:PHE:CD2	1:H:2318:LEU:HA	2.53	0.43
1:L:6145:MET:CB	1:L:6304:LEU:HD11	2.49	0.43
1:A:1257:LYS:HD2	1:A:1320:GLY:N	2.30	0.43
1:A:1218:PHE:HB2	1:A:1244:ILE:HB	1.99	0.43
1:G:1308:LEU:HD21	1:G:1367:PRO:HG3	2.01	0.43
1:E:5329:LEU:HD12	1:E:5329:LEU:N	2.33	0.43
1:B:2463:THR:HG23	4:B:7799:HOH:O	2.18	0.43
1:I:3206:ALA:HA	1:I:3210:GLY:O	2.19	0.43
1:F:6358:LEU:HD23	1:F:6468:HIS:HB3	2.00	0.43
1:I:3480:PHE:HZ	1:I:3494:LYS:CG	2.32	0.43
1:A:1104:ARG:HG2	1:A:1104:ARG:NH1	2.33	0.43
1:I:3227:VAL:O	1:I:3231:VAL:HG23	2.19	0.43
1:C:3447:TYR:HA	1:C:3527:LEU:O	2.19	0.43
1:J:4407:THR:HG21	1:J:4412:LYS:CD	2.47	0.43
1:L:6533:THR:C	1:L:6534:GLN:HG3	2.39	0.43
1:G:1523:LYS:HD3	1:G:1537:GLN:HE22	1.84	0.43
1:E:5064:ARG:O	1:E:5065:PHE:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:6142:GLY:O	3:L:6:N LX:H101	2.18	0.42
1:B:2174:ILE:HD12	1:B:2298:THR:CG2	2.49	0.42
1:G:1360:PRO:HB2	4:G:7264:HOH:O	2.19	0.42
1:F:6351:ASN:N	1:F:6351:ASN:HD22	2.16	0.42
1:C:3023:PRO:HA	1:C:3024:PRO:HD3	1.78	0.42
1:B:2477:GLY:HA2	1:B:2493:SER:OG	2.19	0.42
1:G:1351:ASN:N	1:G:1351:ASN:HD22	2.16	0.42
1:A:1330:LYS:HB2	1:A:1335:LEU:HD21	2.01	0.42
1:G:1119:LEU:HD12	1:G:1119:LEU:O	2.19	0.42
1:H:2341:PHE:HE1	1:H:2437:HIS:ND1	2.17	0.42
1:E:5218:PHE:HB3	1:E:5244:ILE:HB	1.99	0.42
1:B:2290:THR:OG1	1:B:2293:GLU:HG3	2.19	0.42
1:C:3044:ALA:O	1:C:3046:PRO:HD3	2.19	0.42
1:F:6143:GLY:O	1:F:6144:LEU:HB2	2.20	0.42
1:C:3242:ARG:NH1	1:C:3242:ARG:CG	2.77	0.42
1:I:3272:ALA:O	1:I:3289:LYS:HE3	2.19	0.42
1:I:3364:MET:CE	3:I:3:N LX:H171	2.49	0.42
1:I:3420:LEU:HD13	1:I:3547:TRP:HZ2	1.81	0.42
1:A:1086:MET:HE2	1:A:1110:LEU:CD1	2.47	0.42
1:A:1309:GLN:HE21	1:A:1309:GLN:C	2.22	0.42
1:L:6264:LEU:HD22	1:L:6268:ILE:HD13	2.01	0.42
1:K:5057:LYS:HB3	1:K:5069:GLN:HB2	2.01	0.42
1:I:3104:ARG:HG2	1:I:3104:ARG:HH11	1.84	0.42
1:L:6125:ALA:HB2	1:L:6133:LEU:CD1	2.49	0.42
1:L:6185:SER:HB2	1:L:6283:VAL:HG21	2.01	0.42
1:H:2491:ARG:HH11	1:H:2491:ARG:HG2	1.84	0.42
1:F:6125:ALA:HB2	1:F:6133:LEU:CD1	2.49	0.42
1:J:4125:ALA:HB2	1:J:4133:LEU:HD12	2.00	0.42
1:E:5518:PRO:HD3	1:E:5535:ALA:HB2	2.01	0.42
1:E:5359:ILE:HB	1:E:5360:PRO:CD	2.50	0.42
1:A:1304:LEU:CG	3:A:1:N LX:H151	2.49	0.42
1:G:1104:ARG:HD2	1:G:1108:ILE:HG12	2.00	0.42
1:H:2389:VAL:HB	1:H:2424:VAL:HG11	2.00	0.42
1:G:1383:TRP:CE3	1:G:1383:TRP:HA	2.54	0.42
1:J:4119:LEU:C	1:J:4119:LEU:HD12	2.39	0.42
1:C:3034:LEU:C	1:C:3034:LEU:HD13	2.40	0.42
1:B:2257:LYS:HE2	1:B:2316:GLN:HE22	1.84	0.42
1:J:4453:PRO:HD2	1:J:4470:ASP:OD2	2.19	0.42
1:K:5144:LEU:HB3	1:K:5177:PHE:CE2	2.55	0.42
1:D:4188:ASN:HD22	1:D:4324:ASP:CG	2.22	0.42
1:F:6097:LEU:HD23	1:F:6146:VAL:HG23	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2467:ASP:OD1	1:B:2468:HIS:N	2.46	0.42
1:E:5304:LEU:HD22	3:E:5:NLX:C10	2.41	0.42
1:H:2404:LEU:HB3	1:H:2413:LYS:CG	2.38	0.42
1:L:6188:ASN:ND2	1:L:6324:ASP:OD2	2.52	0.42
1:G:1220:GLU:OE2	1:G:1468:HIS:NE2	2.53	0.42
1:J:4374:ASP:O	1:J:4376:LYS:N	2.52	0.42
1:E:5126:ASP:O	1:E:5128:THR:N	2.53	0.42
1:K:5336:GLN:HE22	1:K:5433:VAL:HA	1.84	0.42
1:L:6246:GLU:HG2	1:L:6447:TYR:OH	2.20	0.42
1:E:5309:GLN:NE2	4:E:7812:HOH:O	2.49	0.42
1:B:2308:LEU:HD11	1:B:2367:PRO:CG	2.49	0.42
1:B:2252:THR:HG22	1:B:2254:VAL:HG12	2.01	0.42
1:H:2026:VAL:HG12	1:H:2027:ASP:N	2.34	0.42
1:E:5211:ASN:HD22	1:E:5214:SER:CB	2.32	0.42
1:H:2040:LEU:HD13	1:H:2155:LEU:HD13	2.01	0.42
1:B:2277:THR:HG22	1:B:2278:THR:HG23	2.01	0.42
1:A:1467:ASP:N	1:A:1470:ASP:OD2	2.52	0.42
1:J:4321:THR:HG22	1:J:4322:VAL:N	2.35	0.42
1:A:1098:SER:O	1:A:1102:THR:HB	2.20	0.42
1:J:4363:LEU:HD22	3:J:4:NLX:C19	2.49	0.42
1:A:1404:LEU:O	1:A:1413:LYS:HE2	2.19	0.42
1:L:6290:THR:O	1:L:6291:GLU:C	2.58	0.42
1:J:4132:ARG:HA	1:J:4132:ARG:HD3	1.79	0.42
1:A:1527:LEU:HD11	1:A:1533:THR:HG23	2.00	0.42
1:C:3211:ASN:HA	1:C:3212:PRO:HD2	1.93	0.42
1:F:6023:PRO:HA	1:F:6024:PRO:HD3	1.74	0.42
1:J:4231:VAL:O	1:J:4231:VAL:HG12	2.19	0.42
1:D:4079:ASN:CB	2:D:479:NAG:H82	2.49	0.42
1:F:6108:ILE:HA	1:F:6109:PRO:HD3	1.81	0.42
1:K:5495:MET:HE3	1:K:5529:ILE:HG23	2.01	0.42
1:K:5025:VAL:CG2	1:K:5034:LEU:HD23	2.50	0.42
1:D:4164:VAL:HG11	1:D:4205:ILE:HD11	2.01	0.42
1:B:2367:PRO:C	1:B:2368:LEU:HD12	2.40	0.42
1:C:3140:HIS:CD2	1:C:3147:GLY:HA3	2.54	0.42
1:L:6096:LEU:HD12	1:L:6096:LEU:O	2.19	0.42
1:H:2330:LYS:HB3	1:H:2334:GLU:OE2	2.19	0.42
1:E:5382:LEU:O	1:E:5385:SER:HB2	2.19	0.42
1:J:4480:PHE:HZ	1:J:4494:LYS:HG3	1.83	0.42
1:D:4139:ILE:HG12	1:D:4168:ILE:HD11	2.01	0.42
1:C:3022:SER:N	4:C:7654:HOH:O	2.51	0.42
1:J:4312:PRO:C	1:J:4314:GLU:H	2.23	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1175:TRP:CZ2	1:A:1294:LEU:HB2	2.54	0.42
1:L:6085:PRO:HG2	1:L:6115:ASP:O	2.19	0.42
1:C:3152:TYR:N	1:C:3152:TYR:CD1	2.88	0.42
1:H:2152:TYR:N	1:H:2152:TYR:CD1	2.88	0.42
1:A:1426:PHE:CD1	1:A:1426:PHE:N	2.87	0.42
1:D:4145:MET:HB3	1:D:4304:LEU:HD21	2.00	0.42
1:A:1025:VAL:CG2	1:A:1034:LEU:HD23	2.33	0.42
1:L:6097:LEU:HD13	3:L:6:N LX:O4	2.19	0.42
1:L:6358:LEU:CD1	1:L:6363:LEU:HD11	2.50	0.42
1:B:2104:ARG:CZ	1:B:2108:ILE:HD12	2.50	0.42
1:J:4102:THR:OG1	1:J:4103:ASN:N	2.52	0.42
1:E:5447:TYR:HB3	1:E:5517:TRP:CZ2	2.54	0.42
1:D:4086:MET:SD	1:D:4089:GLN:NE2	2.92	0.42
1:A:1420:LEU:HD12	1:A:1547:TRP:HZ2	1.84	0.42
1:A:1176:GLY:HA2	1:A:1189:TRP:HB2	2.02	0.42
1:F:6492:LEU:O	1:F:6496:VAL:HG23	2.20	0.42
1:H:2119:LEU:O	1:H:2119:LEU:HD12	2.19	0.42
1:G:1372:GLN:HE22	1:L:6463:THR:HB	1.85	0.42
1:K:5197:ALA:O	1:K:5200:TRP:HB3	2.19	0.42
1:J:4190:GLY:O	1:J:4194:GLN:HG3	2.19	0.42
1:L:6040:LEU:HD13	1:L:6155:LEU:HD13	2.01	0.42
1:A:1421:ILE:H	1:A:1421:ILE:HD12	1.85	0.42
1:H:2404:LEU:O	1:H:2413:LYS:HE2	2.20	0.42
1:I:3420:LEU:C	1:I:3420:LEU:HD12	2.40	0.42
1:G:1411:VAL:HG21	1:L:6411:VAL:HG21	2.01	0.42
1:G:1425:MET:HB2	1:G:1426:PHE:CD1	2.54	0.42
1:L:6452:ARG:HB2	1:L:6465:ILE:HA	2.02	0.42
1:I:3366:TYR:OH	1:I:3385:SER:OG	2.33	0.42
1:B:2257:LYS:HD2	1:B:2257:LYS:N	2.34	0.42
1:D:4366:TYR:HA	1:D:4367:PRO:HD3	1.88	0.42
1:I:3332:PRO:O	1:I:3336:GLN:HG3	2.19	0.42
1:I:3138:TRP:CZ3	1:I:3219:GLY:HA2	2.55	0.42
1:F:6086:MET:HB3	1:F:6110:LEU:HD13	2.00	0.42
1:J:4517:TRP:HA	1:J:4518:PRO:HD2	1.91	0.42
1:H:2255:LEU:HD23	1:H:2318:LEU:HD21	2.01	0.42
1:E:5142:GLY:CA	3:E:5:N LX:H82	2.42	0.42
1:L:6105:LYS:HB2	1:L:6481:LEU:O	2.19	0.42
1:K:5395:LEU:HD13	1:K:5550:LEU:CD2	2.50	0.42
1:H:2382:LEU:HA	1:H:2385:SER:OG	2.19	0.42
1:E:5414:LYS:HB3	1:E:5414:LYS:NZ	2.34	0.42
1:H:2316:GLN:HA	1:H:2317:PRO:HD2	1.91	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:6420:LEU:CD1	1:F:6547:TRP:CZ2	3.02	0.42
1:B:2402:LYS:HE2	1:B:2546:PHE:CD1	2.54	0.42
1:J:4107:ASN:ND2	1:J:4108:ILE:N	2.68	0.42
1:I:3268:ILE:HD11	1:I:3319:LEU:HD21	2.01	0.42
1:J:4089:GLN:OE1	1:J:4094:GLY:HA3	2.20	0.42
1:I:3126:ASP:OD1	1:I:3129:LYS:HG3	2.20	0.42
1:K:5061:GLY:HA3	1:K:5062:PRO:HD3	1.79	0.42
1:K:5089:GLN:O	1:K:5090:ASP:C	2.57	0.42
1:C:3343:THR:HB	1:C:3442:ALA:CB	2.42	0.42
1:J:4130:LYS:HE2	1:J:4132:ARG:HE	1.83	0.42
1:K:5420:LEU:O	1:K:5424:VAL:HG23	2.20	0.42
1:L:6375:GLN:HG3	1:L:6400:THR:CG2	2.50	0.42
1:I:3410:THR:HA	1:I:3413:LYS:HB2	2.01	0.42
1:I:3338:GLU:C	1:I:3340:ASN:N	2.71	0.42
1:H:2190:GLY:O	1:H:2194:GLN:HG3	2.19	0.42
1:G:1223:GLY:O	1:G:1227:VAL:HG23	2.19	0.42
1:F:6190:GLY:O	1:F:6193:ASP:HB2	2.20	0.42
1:I:3499:PHE:HD2	1:I:3509:PRO:O	2.03	0.42
1:L:6171:ARG:HD2	1:L:6175:TRP:O	2.20	0.42
1:E:5526:TYR:CE2	1:E:5539:LEU:HB2	2.55	0.42
1:I:3298:THR:HG22	1:I:3298:THR:O	2.20	0.42
1:H:2304:LEU:CG	3:H:2:NLX:H201	2.49	0.42
1:D:4143:GLY:C	1:D:4145:MET:H	2.23	0.42
1:A:1375:GLN:NE2	1:A:1375:GLN:HA	2.35	0.42
1:A:1246:GLU:HG2	1:A:1447:TYR:OH	2.19	0.42
1:L:6545:ALA:HA	1:L:6548:THR:CG2	2.49	0.42
1:C:3444:THR:HG22	1:C:3445:TYR:N	2.35	0.42
1:K:5069:GLN:HE21	1:K:5069:GLN:HA	1.83	0.42
1:H:2311:ASP:HB3	1:H:2314:GLU:CG	2.50	0.42
1:B:2403:TYR:OH	1:B:2423:ASP:OD2	2.30	0.42
1:A:1324:ASP:OD2	1:A:1325:GLY:N	2.52	0.42
1:F:6398:GLU:HB2	4:F:7899:HOH:O	2.18	0.42
1:F:6243:ALA:O	1:F:6346:TYR:HA	2.19	0.42
1:C:3218:PHE:CB	1:C:3244:ILE:HB	2.49	0.42
1:E:5537:GLN:NE2	4:E:7903:HOH:O	2.51	0.42
1:D:4198:LEU:HA	1:D:4198:LEU:HD23	1.84	0.42
1:A:1251:LEU:HD12	1:A:1433:VAL:HG23	2.02	0.41
1:A:1375:GLN:HE21	1:A:1375:GLN:HA	1.85	0.41
1:K:5241:HIS:O	1:K:5345:PRO:HD2	2.20	0.41
1:G:1251:LEU:HB2	1:G:1429:PRO:HB3	2.00	0.41
1:A:1218:PHE:HA	1:A:1244:ILE:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:6064:ARG:HH11	1:F:6287:ARG:HA	1.84	0.41
1:I:3414:LYS:HD2	1:I:3414:LYS:O	2.20	0.41
1:G:1264:LEU:HD11	1:G:1316:GLN:HG2	2.02	0.41
1:E:5087:CYS:O	1:E:5088:THR:C	2.58	0.41
1:A:1049:ILE:HD13	1:A:1122:TYR:CE2	2.55	0.41
1:L:6111:LYS:NZ	4:L:7632:HOH:O	2.49	0.41
1:E:5202:GLN:HG2	4:E:7074:HOH:O	2.19	0.41
1:C:3512:GLU:HB3	4:C:7492:HOH:O	2.19	0.41
1:J:4527:LEU:HD11	1:J:4533:THR:HG22	2.02	0.41
1:F:6453:PRO:HA	1:F:6489:GLU:OE1	2.20	0.41
1:H:2304:LEU:HD22	3:H:2:NLX:H162	2.00	0.41
1:A:1363:LEU:HD22	3:A:1:NLX:C18	2.43	0.41
1:K:5550:LEU:C	1:K:5552:ALA:N	2.74	0.41
1:I:3251:LEU:HD12	1:I:3433:VAL:HG22	2.02	0.41
1:L:6254:VAL:HG12	4:L:7486:HOH:O	2.19	0.41
1:A:1303:PHE:CZ	1:A:1319:LEU:HD11	2.55	0.41
1:C:3427:GLY:O	1:C:3428:VAL:C	2.59	0.41
1:G:1398:GLU:OE1	1:G:1550:LEU:HD13	2.20	0.41
1:F:6420:LEU:CD1	1:F:6547:TRP:HZ2	2.33	0.41
1:G:1381:LEU:HD21	1:L:6459:MET:HB3	2.01	0.41
1:F:6218:PHE:CB	1:F:6244:ILE:HB	2.50	0.41
1:L:6420:LEU:HD11	1:L:6547:TRP:CH2	2.55	0.41
1:I:3023:PRO:HA	1:I:3024:PRO:HD3	1.68	0.41
1:K:5333:GLU:OE1	1:K:5333:GLU:N	2.31	0.41
1:K:5493:SER:O	1:K:5497:MET:HG3	2.20	0.41
1:F:6445:TYR:CE1	1:F:6509:PRO:HD2	2.55	0.41
1:E:5225:GLU:O	1:E:5228:SER:HB3	2.19	0.41
1:I:3091:PRO:HB3	1:I:3112:LEU:HD11	2.02	0.41
1:F:6262:LYS:HA	1:F:6262:LYS:HD2	1.90	0.41
1:K:5438:ARG:HD2	1:K:5522:GLN:NE2	2.35	0.41
1:H:2368:LEU:O	1:K:5368:LEU:O	2.38	0.41
1:E:5221:SER:HB2	3:E:5:NLX:O3	2.19	0.41
1:G:1145:MET:CG	1:G:1304:LEU:HD21	2.50	0.41
1:K:5051:LEU:HD22	1:K:5083:TYR:CE1	2.55	0.41
1:A:1246:GLU:HB3	1:A:1471:GLU:OE1	2.20	0.41
1:E:5372:GLN:HB3	1:E:5410:THR:OG1	2.20	0.41
1:D:4079:ASN:CG	2:D:479:NAG:C1	2.88	0.41
1:G:1244:ILE:HD11	1:G:1503:PHE:CD2	2.55	0.41
1:G:1435:ARG:NH2	1:G:1541:ASP:OD2	2.53	0.41
1:I:3220:GLU:HA	1:I:3246:GLU:O	2.20	0.41
1:K:5540:LYS:HA	1:K:5543:GLU:OE2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1367:PRO:O	1:G:1368:LEU:HD23	2.20	0.41
1:D:4317:PRO:O	1:D:4318:LEU:HB3	2.20	0.41
1:K:5404:LEU:HD22	1:K:5413:LYS:O	2.20	0.41
1:K:5480:PHE:N	1:K:5480:PHE:CD1	2.88	0.41
1:A:1526:TYR:CZ	1:A:1536:ALA:HB3	2.55	0.41
1:K:5401:GLU:O	1:K:5402:LYS:C	2.58	0.41
1:L:6383:TRP:HA	1:L:6383:TRP:CE3	2.55	0.41
1:C:3304:LEU:HA	3:C:3:NLX:H201	2.02	0.41
1:B:2237:LYS:HA	1:B:2237:LYS:HD3	1.89	0.41
1:H:2176:GLY:O	1:H:2189:TRP:N	2.53	0.41
1:E:5487:GLU:HG3	1:E:5491:ARG:CZ	2.50	0.41
1:K:5290:THR:HG23	1:K:5293:GLU:OE2	2.20	0.41
1:L:6375:GLN:HA	1:L:6378:ALA:HB3	2.01	0.41
1:G:1170:TYR:CD1	1:G:1170:TYR:N	2.89	0.41
1:L:6412:LYS:O	1:L:6416:LEU:HD12	2.20	0.41
1:C:3348:VAL:O	1:C:3446:MET:HA	2.20	0.41
1:D:4040:LEU:O	1:D:4041:GLU:C	2.57	0.41
1:G:1448:GLU:OE2	1:G:1539:LEU:CD1	2.69	0.41
1:D:4351:ASN:ND2	1:D:4449:PHE:HB3	2.35	0.41
1:C:3366:TYR:HA	1:C:3367:PRO:HD3	1.79	0.41
1:D:4486:SER:HB2	1:D:4489:GLU:H	1.84	0.41
1:J:4296:GLU:O	1:J:4300:LYS:HG3	2.20	0.41
1:K:5255:LEU:O	1:K:5320:GLY:HA3	2.21	0.41
1:J:4524:GLU:HG3	1:J:4538:LYS:CE	2.50	0.41
1:D:4442:ALA:HA	1:D:4443:PRO:HD3	1.87	0.41
1:L:6363:LEU:CB	3:L:6:NLX:H162	2.48	0.41
1:L:6093:ALA:CB	3:L:6:NLX:H192	2.50	0.41
1:A:1153:ASP:OD2	1:A:1153:ASP:C	2.59	0.41
1:A:1373:LEU:N	1:A:1373:LEU:HD12	2.36	0.41
1:E:5290:THR:HG23	1:E:5293:GLU:OE2	2.21	0.41
1:G:1452:ARG:HA	1:G:1453:PRO:HD2	1.85	0.41
1:I:3389:VAL:HG23	1:I:3391:ILE:HG13	2.03	0.41
1:C:3104:ARG:NH1	1:C:3153:ASP:HB2	2.36	0.41
1:B:2423:ASP:HA	4:B:7059:HOH:O	2.19	0.41
1:B:2161:GLU:HG3	1:B:2501:ALA:CB	2.51	0.41
1:G:1045:GLN:NE2	1:G:1046:PRO:HD2	2.35	0.41
1:H:2345:PRO:HA	1:H:2443:PRO:O	2.20	0.41
1:G:1345:PRO:HA	1:G:1443:PRO:O	2.21	0.41
1:H:2097:LEU:CD1	3:H:2:NLX:H11	2.51	0.41
1:F:6096:LEU:HD23	1:F:6363:LEU:HD21	2.03	0.41
1:I:3289:LYS:HA	1:I:3293:GLU:OE2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:3304:LEU:HA	3:I:3:NLX:H202	2.01	0.41
1:I:3364:MET:SD	3:I:3:NLX:H171	2.61	0.41
1:E:5321:THR:HG22	1:E:5322:VAL:N	2.35	0.41
1:E:5395:LEU:HD13	1:E:5550:LEU:CD1	2.50	0.41
1:J:4232:LEU:HA	1:J:4341:PHE:HB3	2.02	0.41
1:K:5252:THR:HG23	1:K:5425:MET:O	2.21	0.41
1:F:6047:VAL:HG21	1:F:6155:LEU:CD2	2.48	0.41
1:E:5105:LYS:HZ2	1:E:5482:LYS:HA	1.86	0.41
1:L:6311:ASP:OD1	1:L:6313:ARG:N	2.49	0.41
1:G:1119:LEU:HD12	1:G:1119:LEU:C	2.41	0.41
1:A:1186:ARG:HB3	1:A:1324:ASP:HB2	2.03	0.41
1:D:4279:SER:O	1:D:4283:VAL:HG23	2.21	0.41
1:H:2074:TRP:CE2	1:H:2078:LYS:HD2	2.55	0.41
1:H:2354:GLU:O	1:H:2468:HIS:HB2	2.20	0.41
1:A:1398:GLU:OE2	1:A:1550:LEU:HD13	2.20	0.41
1:D:4145:MET:CB	1:D:4304:LEU:HD21	2.51	0.41
1:A:1447:TYR:HB3	1:A:1517:TRP:CZ2	2.55	0.41
1:H:2107:ASN:ND2	1:H:2108:ILE:N	2.68	0.41
1:C:3386:TYR:N	1:C:3387:PRO:HD2	2.35	0.41
1:C:3449:PHE:CE2	1:C:3451:TYR:HB3	2.55	0.41
1:C:3526:TYR:CD2	1:C:3539:LEU:HB2	2.55	0.41
1:H:2103:ASN:O	1:H:2481:LEU:HB2	2.21	0.41
1:C:3355:PHE:CD1	1:C:3421:ILE:HG21	2.56	0.41
1:I:3112:LEU:O	1:I:3113:SER:HB2	2.20	0.41
1:I:3043:PHE:N	1:I:3043:PHE:CD1	2.88	0.41
1:J:4211:ASN:HA	1:J:4212:PRO:HD2	1.94	0.41
1:D:4325:GLY:O	1:D:4329:LEU:CD2	2.69	0.41
1:L:6546:PHE:O	1:L:6549:ASN:HB3	2.20	0.41
1:D:4275:LYS:HD3	1:D:4275:LYS:HA	1.73	0.41
1:H:2358:LEU:HG	1:H:2363:LEU:HD12	2.03	0.41
1:L:6090:ASP:HB3	1:L:6093:ALA:HB3	2.03	0.41
1:I:3498:LYS:HB3	1:I:3514:LEU:CD1	2.47	0.41
1:A:1367:PRO:HB3	1:F:6361:MET:HG2	2.02	0.41
1:G:1354:GLU:OE1	1:G:1354:GLU:HA	2.20	0.41
1:A:1140:HIS:HD2	1:A:1141:GLY:O	2.03	0.41
1:G:1352:LYS:HD3	1:G:1450:GLN:CD	2.41	0.41
1:A:1420:LEU:HD12	1:A:1547:TRP:CZ2	2.55	0.41
1:F:6451:TYR:HE2	1:F:6489:GLU:HG3	1.86	0.41
1:C:3205:ILE:HA	1:C:3205:ILE:HD12	1.95	0.41
1:G:1311:ASP:HA	1:G:1312:PRO:HD3	1.90	0.41
1:L:6393:LYS:O	1:L:6396:ILE:HG12	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:2464:VAL:HG12	1:H:2467:ASP:HB2	2.03	0.41
1:B:2381:LEU:O	1:B:2384:LYS:N	2.53	0.41
1:F:6336:GLN:O	1:F:6339:ARG:HD2	2.21	0.41
1:D:4375:GLN:HE21	1:D:4375:GLN:HB3	1.50	0.41
1:C:3143:GLY:CA	3:C:3:NLX:C15	2.94	0.41
1:J:4363:LEU:HD22	3:J:4:NLX:C18	2.51	0.41
1:L:6304:LEU:HB3	3:L:6:NLX:C17	2.51	0.41
1:G:1428:VAL:CB	1:G:1429:PRO:HD3	2.46	0.41
1:E:5491:ARG:HG2	1:E:5491:ARG:NH1	2.36	0.41
1:A:1104:ARG:NH1	1:A:1153:ASP:OD1	2.54	0.41
1:A:1220:GLU:O	1:A:1221:SER:HB3	2.21	0.41
1:L:6140:HIS:CD2	1:L:6141:GLY:N	2.89	0.41
1:L:6375:GLN:O	1:L:6378:ALA:HB3	2.21	0.41
1:G:1395:LEU:HD22	1:G:1550:LEU:HD12	2.03	0.41
1:E:5375:GLN:HE22	1:E:5401:GLU:HA	1.85	0.41
1:I:3473:PHE:HB3	1:I:3478:ALA:HB3	2.02	0.41
1:K:5527:LEU:HG	1:K:5529:ILE:HG13	2.03	0.41
1:K:5034:LEU:HD13	1:K:5034:LEU:O	2.21	0.41
1:J:4447:TYR:C	1:J:4447:TYR:CD2	2.94	0.41
1:C:3534:GLN:N	1:C:3534:GLN:CD	2.73	0.41
1:I:3277:THR:HG22	1:I:3278:THR:HG23	2.03	0.41
1:G:1132:ARG:HD3	1:G:1132:ARG:HA	1.80	0.41
1:K:5217:ILE:HG13	1:K:5227:VAL:HG13	2.03	0.41
1:H:2409:ASP:C	1:H:2411:VAL:H	2.25	0.41
1:E:5455:PHE:CE1	1:E:5478:ALA:HB3	2.56	0.41
1:L:6444:THR:HG22	1:L:6445:TYR:N	2.35	0.41
1:L:6218:PHE:HB2	1:L:6244:ILE:HB	2.03	0.41
1:A:1417:PHE:O	1:A:1420:LEU:HB3	2.21	0.41
1:C:3475:VAL:HG22	1:C:3496:VAL:CG1	2.50	0.41
1:K:5404:LEU:C	1:K:5406:GLY:H	2.23	0.41
1:A:1126:ASP:OD2	1:A:1129:LYS:HG2	2.21	0.41
1:F:6262:LYS:NZ	1:F:6282:MET:CE	2.84	0.41
1:D:4488:GLU:HG2	1:D:4489:GLU:N	2.35	0.41
1:G:1402:LYS:HG3	1:G:1402:LYS:O	2.20	0.41
1:I:3177:PHE:N	1:I:3177:PHE:CD2	2.89	0.41
1:J:4351:ASN:HB3	1:J:4466:GLY:O	2.21	0.41
1:C:3055:PHE:CE1	1:C:3197:ALA:HB2	2.56	0.41
1:C:3175:TRP:CZ2	1:C:3294:LEU:HB2	2.56	0.41
1:C:3067:PRO:HB3	1:C:3192:LEU:HD13	2.03	0.41
1:A:1494:LYS:O	1:A:1498:LYS:HB2	2.21	0.41
1:E:5145:MET:CG	1:E:5318:LEU:HD23	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:6:N LX:H203	3:L:6:N LX:O4	2.21	0.41
1:C:3371:GLY:HA2	1:D:4371:GLY:HA3	2.02	0.41
1:E:5257:LYS:HE3	1:E:5316:GLN:OE1	2.20	0.41
1:J:4455:PHE:CE2	1:J:4482:LYS:HB2	2.56	0.41
1:E:5237:LYS:HZ2	1:E:5340:ASN:ND2	2.19	0.41
1:C:3104:ARG:HH11	1:C:3104:ARG:HG2	1.86	0.41
1:L:6452:ARG:HA	1:L:6453:PRO:HD2	1.95	0.41
1:A:1205:ILE:HA	1:A:1205:ILE:HD12	1.92	0.41
1:E:5493:SER:O	1:E:5497:MET:HG3	2.21	0.41
1:F:6359:ILE:HG23	3:F:6:N LX:H161	2.03	0.40
1:A:1257:LYS:NZ	1:A:1318:LEU:O	2.49	0.40
1:F:6330:LYS:HB2	1:F:6334:GLU:OE1	2.20	0.40
1:F:6338:GLU:C	1:F:6340:ASN:N	2.72	0.40
1:I:3354:GLU:HB2	1:I:3422:ALA:HB1	2.04	0.40
1:D:4079:ASN:ND2	4:D:7835:HOH:O	2.48	0.40
1:K:5313:ARG:HA	1:K:5386:TYR:CD2	2.57	0.40
1:J:4313:ARG:HG2	1:J:4386:TYR:CE2	2.57	0.40
1:L:6048:ALA:HB3	1:L:6123:THR:CG2	2.50	0.40
1:L:6382:LEU:HD21	1:L:6420:LEU:HD21	2.02	0.40
1:D:4057:LYS:HG3	1:D:4058:PRO:HD2	2.03	0.40
1:E:5346:TYR:HB3	1:E:5437:HIS:CD2	2.56	0.40
1:L:6452:ARG:NH1	1:L:6452:ARG:HG2	2.36	0.40
1:G:1149:ALA:CB	1:G:1169:GLN:HG3	2.51	0.40
1:B:2549:ASN:O	1:B:2552:ALA:N	2.52	0.40
1:H:2435:ARG:O	1:H:2438:ARG:HB3	2.22	0.40
1:D:4030:HIS:CD2	1:D:4071:ALA:HB3	2.56	0.40
1:I:3107:ASN:HD22	1:I:3108:ILE:H	1.69	0.40
1:F:6303:PHE:HB3	1:F:6317:PRO:O	2.21	0.40
1:J:4138:TRP:CH2	1:J:4220:GLU:HB2	2.57	0.40
1:J:4303:PHE:C	1:J:4304:LEU:HD22	2.41	0.40
1:A:1349:GLY:HA3	1:A:1447:TYR:CD1	2.56	0.40
1:A:1449:PHE:CE2	1:A:1471:GLU:HA	2.56	0.40
1:I:3087:CYS:O	1:I:3088:THR:C	2.59	0.40
1:L:6104:ARG:HD2	4:L:7255:HOH:O	2.22	0.40
1:C:3495:MET:HG3	1:C:3514:LEU:CD2	2.49	0.40
1:H:2428:VAL:HB	1:H:2429:PRO:HD3	2.03	0.40
1:B:2241:HIS:O	1:B:2242:ARG:HD2	2.21	0.40
1:G:1517:TRP:CE3	1:G:1527:LEU:HD22	2.56	0.40
1:D:4370:GLU:HA	1:D:4370:GLU:OE2	2.22	0.40
1:D:4338:GLU:H	1:D:4338:GLU:HG3	1.54	0.40
1:D:4455:PHE:CD2	1:D:4482:LYS:HD3	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:5205:ILE:HA	1:K:5205:ILE:HD12	1.88	0.40
1:A:1254:VAL:O	1:A:1254:VAL:HG22	2.22	0.40
1:B:2373:LEU:CD2	1:B:2378:ALA:HB2	2.33	0.40
1:E:5221:SER:HA	1:E:5247:SER:O	2.21	0.40
1:L:6358:LEU:HD11	1:L:6363:LEU:HD11	2.04	0.40
1:K:5318:LEU:HD11	3:K:5:N LX:C2	2.52	0.40
1:K:5357:TRP:O	1:K:5361:MET:CB	2.69	0.40
1:G:1221:SER:OG	1:G:1222:ALA:N	2.53	0.40
1:I:3359:ILE:HG23	3:I:3:N LX:C15	2.51	0.40
1:I:3452:ARG:CZ	1:I:3462:LYS:HA	2.52	0.40
1:C:3223:GLY:O	1:C:3227:VAL:HG23	2.22	0.40
1:A:1229:VAL:O	1:A:1232:LEU:N	2.51	0.40
1:A:1316:GLN:HA	1:A:1316:GLN:OE1	2.21	0.40
1:K:5425:MET:HG2	4:K:7147:HOH:O	2.22	0.40
1:H:2264:LEU:HD22	1:H:2316:GLN:HG3	2.02	0.40
1:K:5495:MET:O	1:K:5499:PHE:HB2	2.22	0.40
1:I:3151:THR:HB	1:I:3152:TYR:CE1	2.55	0.40
1:C:3464:VAL:CG2	1:D:4370:GLU:HG3	2.51	0.40
1:F:6191:HIS:CD2	1:F:6321:THR:HG23	2.56	0.40
1:F:6342:HIS:CD2	4:F:7231:HOH:O	2.74	0.40
1:F:6074:TRP:NE1	1:F:6078:LYS:HB2	2.36	0.40
1:H:2091:PRO:HG3	1:H:2112:LEU:HD11	2.04	0.40
1:C:3040:LEU:HD13	1:C:3155:LEU:HD13	2.03	0.40
1:B:2205:ILE:HG13	1:B:2210:GLY:HA3	2.02	0.40
1:J:4061:GLY:HA2	4:J:8043:HOH:O	2.21	0.40
1:A:1123:THR:HG23	1:A:1123:THR:O	2.21	0.40
1:E:5145:MET:CB	1:E:5304:LEU:HD11	2.49	0.40
1:H:2048:ALA:HB3	1:H:2123:THR:CG2	2.47	0.40
1:L:6263:PRO:HB2	4:L:7197:HOH:O	2.21	0.40
1:K:5450:GLN:O	1:K:5451:TYR:HB2	2.21	0.40
1:L:6545:ALA:C	1:L:6548:THR:HG22	2.42	0.40
1:K:5498:LYS:HG2	1:K:5502:ASN:ND2	2.33	0.40
1:A:1341:PHE:N	1:A:1341:PHE:CD2	2.89	0.40
1:D:4211:ASN:HA	1:D:4212:PRO:HD2	1.93	0.40
1:K:5249:VAL:H	1:K:5252:THR:HG1	1.70	0.40
1:J:4370:GLU:C	1:J:4372:GLN:H	2.24	0.40
1:C:3431:VAL:HA	1:C:3446:MET:CE	2.51	0.40
1:A:1539:LEU:N	4:A:7558:HOH:O	2.54	0.40
1:G:1351:ASN:O	1:G:1352:LYS:C	2.60	0.40
1:J:4182:ASP:N	1:J:4182:ASP:OD2	2.54	0.40
1:I:3191:HIS:HD2	1:I:3321:THR:HG23	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:2244:ILE:HG12	1:H:2347:MET:HB3	2.03	0.40
1:L:6351:ASN:HD22	1:L:6351:ASN:N	2.19	0.40
1:F:6449:PHE:CE2	1:F:6451:TYR:HB3	2.57	0.40
1:F:6534:GLN:CD	1:F:6534:GLN:H	2.24	0.40
1:F:6471:GLU:O	1:F:6475:VAL:HG23	2.21	0.40
1:A:1519:GLU:HG2	1:A:1520:TYR:N	2.36	0.40
1:E:5022:SER:HB3	4:E:8085:HOH:O	2.21	0.40
1:A:1266:GLU:O	1:A:1270:ILE:HD12	2.21	0.40
1:J:4049:ILE:HG12	1:J:4122:TYR:CD2	2.56	0.40
1:B:2026:VAL:CG1	1:B:2027:ASP:N	2.84	0.40
1:C:3357:TRP:C	1:C:3360:PRO:HD2	2.41	0.40
1:K:5142:GLY:CA	3:K:5:N LX:H82	2.52	0.40
1:J:4428:VAL:CB	1:J:4429:PRO:HD3	2.43	0.40
1:K:5389:VAL:HB	1:K:5391:ILE:HG13	2.03	0.40
1:H:2420:LEU:CD1	1:H:2547:TRP:HZ2	2.33	0.40
1:L:6426:PHE:C	1:L:6429:PRO:HD2	2.42	0.40
1:C:3526:TYR:CE1	1:C:3539:LEU:HD13	2.57	0.40
1:E:5034:LEU:C	1:E:5034:LEU:CD2	2.90	0.40
1:A:1420:LEU:CD1	1:A:1547:TRP:HZ2	2.35	0.40
1:A:1420:LEU:CD1	1:A:1547:TRP:CZ2	3.05	0.40
1:F:6185:SER:HB2	1:F:6283:VAL:HG21	2.03	0.40
1:A:1401:GLU:C	1:A:1403:TYR:H	2.25	0.40
1:B:2339:ARG:O	1:B:2341:PHE:CD2	2.74	0.40
1:K:5036:LYS:HG2	1:K:5049:ILE:HB	2.03	0.40
1:J:4355:PHE:HB2	1:J:4422:ALA:HB2	2.02	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	530/548 (97%)	480 (91%)	41 (8%)	9 (2%)	11 38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	530/548 (97%)	476 (90%)	48 (9%)	6 (1%)	17	51
1	C	529/548 (96%)	489 (92%)	33 (6%)	7 (1%)	15	46
1	D	531/548 (97%)	491 (92%)	36 (7%)	4 (1%)	24	60
1	E	529/548 (96%)	482 (91%)	40 (8%)	7 (1%)	15	46
1	F	529/548 (96%)	477 (90%)	44 (8%)	8 (2%)	13	42
1	G	530/548 (97%)	467 (88%)	55 (10%)	8 (2%)	13	42
1	H	529/548 (96%)	470 (89%)	52 (10%)	7 (1%)	15	46
1	I	529/548 (96%)	466 (88%)	56 (11%)	7 (1%)	15	46
1	J	530/548 (97%)	484 (91%)	40 (8%)	6 (1%)	17	51
1	K	529/548 (96%)	475 (90%)	48 (9%)	6 (1%)	17	51
1	L	529/548 (96%)	467 (88%)	53 (10%)	9 (2%)	11	38
All	All	6354/6576 (97%)	5724 (90%)	546 (9%)	84 (1%)	15	46

All (84) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1253	SER
1	B	2342	HIS
1	C	3253	SER
1	D	4185	SER
1	D	4253	SER
1	E	5237	LYS
1	E	5253	SER
1	G	1253	SER
1	G	1339	ARG
1	G	1375	GLN
1	H	2205	ILE
1	I	3535	ALA
1	J	4105	LYS
1	J	4253	SER
1	L	6539	LEU
1	A	1185	SER
1	A	1375	GLN
1	B	2237	LYS
1	B	2253	SER
1	B	2340	ASN
1	C	3185	SER
1	C	3405	GLY

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Mol	Chain	Res	Type
1	C	3427	GLY
1	D	4552	ALA
1	E	5127	LEU
1	E	5371	GLY
1	F	6185	SER
1	F	6406	GLY
1	G	1462	LYS
1	G	1520	TYR
1	H	2185	SER
1	H	2253	SER
1	H	2375	GLN
1	I	3341	PHE
1	J	4185	SER
1	J	4375	GLN
1	K	5237	LYS
1	K	5340	ASN
1	L	6127	LEU
1	A	1358	LEU
1	C	3127	LEU
1	D	4337	ALA
1	E	5044	ALA
1	F	6357	TRP
1	G	1378	ALA
1	I	3185	SER
1	J	4343	THR
1	J	4371	GLY
1	K	5185	SER
1	K	5253	SER
1	K	5338	GLU
1	L	6142	GLY
1	A	1221	SER
1	A	1406	GLY
1	C	3079	ASN
1	C	3113	SER
1	E	5185	SER
1	F	6253	SER
1	F	6479	PRO
1	G	1185	SER
1	H	2343	THR
1	H	2462	LYS
1	I	3205	ILE
1	L	6041	GLU

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Mol	Chain	Res	Type
1	L	6253	SER
1	L	6254	VAL
1	A	1155	LEU
1	A	1538	LYS
1	B	2044	ALA
1	B	2373	LEU
1	F	6129	LYS
1	G	1352	LYS
1	I	3142	GLY
1	L	6358	LEU
1	L	6538	LYS
1	A	1356	GLY
1	F	6259	GLY
1	F	6358	LEU
1	L	6303	PHE
1	E	5427	GLY
1	I	3367	PRO
1	I	3427	GLY
1	K	5061	GLY
1	H	2173	GLY

### 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	448/463 (97%)	435 (97%)	13 (3%)	50	83
1	B	448/463 (97%)	431 (96%)	17 (4%)	40	76
1	C	447/463 (96%)	420 (94%)	27 (6%)	24	57
1	D	448/463 (97%)	423 (94%)	25 (6%)	26	60
1	E	447/463 (96%)	422 (94%)	25 (6%)	26	60
1	F	447/463 (96%)	426 (95%)	21 (5%)	32	68
1	G	448/463 (97%)	419 (94%)	29 (6%)	21	52
1	H	447/463 (96%)	427 (96%)	20 (4%)	34	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	447/463 (96%)	418 (94%)	29 (6%)	21	52
1	J	448/463 (97%)	426 (95%)	22 (5%)	31	67
1	K	447/463 (96%)	421 (94%)	26 (6%)	25	58
1	L	447/463 (96%)	433 (97%)	14 (3%)	47	82
All	All	5369/5556 (97%)	5101 (95%)	268 (5%)	30	65

All (268) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1078	LYS
1	A	1218	PHE
1	A	1253	SER
1	A	1264	LEU
1	A	1304	LEU
1	A	1309	GLN
1	A	1341	PHE
1	A	1366	TYR
1	A	1394	GLU
1	A	1408	ASP
1	A	1410	THR
1	A	1488	GLU
1	A	1491	ARG
1	B	2034	LEU
1	B	2111	LYS
1	B	2160	HIS
1	B	2218	PHE
1	B	2220	GLU
1	B	2225	GLU
1	B	2258	LYS
1	B	2299	LEU
1	B	2309	GLN
1	B	2319	LEU
1	B	2341	PHE
1	B	2346	TYR
1	B	2366	TYR
1	B	2404	LEU
1	B	2420	LEU
1	B	2499	PHE
1	B	2512	GLU
1	C	3027	ASP
1	C	3088	THR

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Mol	Chain	Res	Type
1	C	3106	GLU
1	C	3107	ASN
1	C	3155	LEU
1	C	3218	PHE
1	C	3220	GLU
1	C	3221	SER
1	C	3225	GLU
1	C	3242	ARG
1	C	3264	LEU
1	C	3296	GLU
1	C	3299	LEU
1	C	3309	GLN
1	C	3319	LEU
1	C	3330	LYS
1	C	3333	GLU
1	C	3339	ARG
1	C	3355	PHE
1	C	3374	ASP
1	C	3394	GLU
1	C	3414	LYS
1	C	3420	LEU
1	C	3483	GLU
1	C	3499	PHE
1	C	3500	TRP
1	C	3534	GLN
1	D	4027	ASP
1	D	4078	LYS
1	D	4106	GLU
1	D	4107	ASN
1	D	4218	PHE
1	D	4242	ARG
1	D	4253	SER
1	D	4264	LEU
1	D	4279	SER
1	D	4304	LEU
1	D	4309	GLN
1	D	4316	GLN
1	D	4327	LEU
1	D	4338	GLU
1	D	4341	PHE
1	D	4346	TYR
1	D	4363	LEU

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Mol	Chain	Res	Type
1	D	4366	TYR
1	D	4372	GLN
1	D	4375	GLN
1	D	4420	LEU
1	D	4458	ASP
1	D	4471	GLU
1	D	4488	GLU
1	D	4491	ARG
1	E	5033	VAL
1	E	5034	LEU
1	E	5079	ASN
1	E	5105	LYS
1	E	5107	ASN
1	E	5111	LYS
1	E	5155	LEU
1	E	5203	ASP
1	E	5218	PHE
1	E	5220	GLU
1	E	5225	GLU
1	E	5258	LYS
1	E	5266	GLU
1	E	5289	LYS
1	E	5305	SER
1	E	5319	LEU
1	E	5340	ASN
1	E	5346	TYR
1	E	5366	TYR
1	E	5370	GLU
1	E	5394	GLU
1	E	5408	ASP
1	E	5463	THR
1	E	5499	PHE
1	E	5500	TRP
1	F	6072	GLU
1	F	6155	LEU
1	F	6203	ASP
1	F	6214	SER
1	F	6220	GLU
1	F	6221	SER
1	F	6249	VAL
1	F	6257	LYS
1	F	6258	LYS

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Mol	Chain	Res	Type
1	F	6264	LEU
1	F	6277	THR
1	F	6323	ILE
1	F	6346	TYR
1	F	6372	GLN
1	F	6374	ASP
1	F	6414	LYS
1	F	6471	GLU
1	F	6489	GLU
1	F	6500	TRP
1	F	6534	GLN
1	F	6541	ASP
1	G	1034	LEU
1	G	1041	GLU
1	G	1104	ARG
1	G	1126	ASP
1	G	1128	THR
1	G	1146	VAL
1	G	1218	PHE
1	G	1225	GLU
1	G	1226	SER
1	G	1264	LEU
1	G	1267	GLN
1	G	1276	THR
1	G	1277	THR
1	G	1279	SER
1	G	1309	GLN
1	G	1318	LEU
1	G	1319	LEU
1	G	1340	ASN
1	G	1346	TYR
1	G	1366	TYR
1	G	1375	GLN
1	G	1380	SER
1	G	1393	LYS
1	G	1407	THR
1	G	1458	ASP
1	G	1463	THR
1	G	1500	TRP
1	G	1522	GLN
1	G	1541	ASP
1	H	2034	LEU

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Mol	Chain	Res	Type
1	H	2111	LYS
1	H	2129	LYS
1	H	2132	ARG
1	H	2155	LEU
1	H	2218	PHE
1	H	2225	GLU
1	H	2258	LYS
1	H	2292	GLU
1	H	2309	GLN
1	H	2338	GLU
1	H	2342	HIS
1	H	2346	TYR
1	H	2404	LEU
1	H	2409	ASP
1	H	2411	VAL
1	H	2483	GLU
1	H	2499	PHE
1	H	2500	TRP
1	H	2532	ASN
1	I	3034	LEU
1	I	3064	ARG
1	I	3072	GLU
1	I	3105	LYS
1	I	3107	ASN
1	I	3155	LEU
1	I	3218	PHE
1	I	3220	GLU
1	I	3225	GLU
1	I	3240	PHE
1	I	3258	LYS
1	I	3264	LEU
1	I	3296	GLU
1	I	3299	LEU
1	I	3330	LYS
1	I	3340	ASN
1	I	3341	PHE
1	I	3346	TYR
1	I	3372	GLN
1	I	3374	ASP
1	I	3385	SER
1	I	3414	LYS
1	I	3420	LEU

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Mol	Chain	Res	Type
1	I	3447	TYR
1	I	3470	ASP
1	I	3500	TRP
1	I	3512	GLU
1	I	3534	GLN
1	I	3549	ASN
1	J	4027	ASP
1	J	4034	LEU
1	J	4041	GLU
1	J	4072	GLU
1	J	4102	THR
1	J	4104	ARG
1	J	4107	ASN
1	J	4218	PHE
1	J	4258	LYS
1	J	4264	LEU
1	J	4282	MET
1	J	4297	THR
1	J	4304	LEU
1	J	4316	GLN
1	J	4319	LEU
1	J	4342	HIS
1	J	4366	TYR
1	J	4375	GLN
1	J	4394	GLU
1	J	4404	LEU
1	J	4471	GLU
1	J	4506	ASN
1	K	5033	VAL
1	K	5066	THR
1	K	5069	GLN
1	K	5128	THR
1	K	5155	LEU
1	K	5220	GLU
1	K	5225	GLU
1	K	5240	PHE
1	K	5242	ARG
1	K	5258	LYS
1	K	5299	LEU
1	K	5305	SER
1	K	5309	GLN
1	K	5330	LYS

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Mol	Chain	Res	Type
1	K	5341	PHE
1	K	5366	TYR
1	K	5374	ASP
1	K	5375	GLN
1	K	5390	CYS
1	K	5426	PHE
1	K	5439	ASP
1	K	5463	THR
1	K	5499	PHE
1	K	5500	TRP
1	K	5512	GLU
1	K	5541	ASP
1	L	6107	ASN
1	L	6130	LYS
1	L	6155	LEU
1	L	6218	PHE
1	L	6220	GLU
1	L	6258	LYS
1	L	6264	LEU
1	L	6278	THR
1	L	6414	LYS
1	L	6419	ASP
1	L	6420	LEU
1	L	6447	TYR
1	L	6463	THR
1	L	6500	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (177) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1030	HIS
1	A	1079	ASN
1	A	1095	GLN
1	A	1131	ASN
1	A	1140	HIS
1	A	1160	HIS
1	A	1162	ASN
1	A	1184	HIS
1	A	1238	ASN
1	A	1241	HIS
1	A	1288	GLN
1	A	1309	GLN

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Mol	Chain	Res	Type
1	A	1336	GLN
1	A	1340	ASN
1	A	1342	HIS
1	A	1351	ASN
1	A	1353	GLN
1	A	1372	GLN
1	A	1375	GLN
1	A	1436	ASN
1	A	1502	ASN
1	B	2030	HIS
1	B	2045	GLN
1	B	2069	GLN
1	B	2140	HIS
1	B	2162	ASN
1	B	2241	HIS
1	B	2309	GLN
1	B	2316	GLN
1	B	2336	GLN
1	B	2351	ASN
1	B	2353	GLN
1	B	2372	GLN
1	B	2436	ASN
1	B	2450	GLN
1	B	2532	ASN
1	B	2537	GLN
1	C	3045	GLN
1	C	3095	GLN
1	C	3140	HIS
1	C	3162	ASN
1	C	3202	GLN
1	C	3238	ASN
1	C	3241	HIS
1	C	3351	ASN
1	C	3353	GLN
1	C	3375	GLN
1	C	3436	ASN
1	C	3437	HIS
1	C	3450	GLN
1	C	3532	ASN
1	C	3534	GLN
1	C	3537	GLN
1	D	4069	GLN

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Mol	Chain	Res	Type
1	D	4107	ASN
1	D	4131	ASN
1	D	4140	HIS
1	D	4241	HIS
1	D	4309	GLN
1	D	4336	GLN
1	D	4342	HIS
1	D	4351	ASN
1	D	4372	GLN
1	D	4375	GLN
1	D	4450	GLN
1	D	4508	ASN
1	D	4510	ASN
1	D	4537	GLN
1	E	5131	ASN
1	E	5140	HIS
1	E	5162	ASN
1	E	5211	ASN
1	E	5241	HIS
1	E	5309	GLN
1	E	5336	GLN
1	E	5340	ASN
1	E	5353	GLN
1	E	5375	GLN
1	E	5436	ASN
1	E	5437	HIS
1	E	5506	ASN
1	E	5532	ASN
1	E	5537	GLN
1	F	6030	HIS
1	F	6079	ASN
1	F	6095	GLN
1	F	6140	HIS
1	F	6160	HIS
1	F	6211	ASN
1	F	6241	HIS
1	F	6336	GLN
1	F	6351	ASN
1	F	6353	GLN
1	F	6436	ASN
1	F	6532	ASN
1	F	6534	GLN

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Mol	Chain	Res	Type
1	G	1045	GLN
1	G	1107	ASN
1	G	1131	ASN
1	G	1140	HIS
1	G	1211	ASN
1	G	1241	HIS
1	G	1267	GLN
1	G	1309	GLN
1	G	1340	ASN
1	G	1351	ASN
1	G	1372	GLN
1	G	1375	GLN
1	G	1436	ASN
1	G	1522	GLN
1	G	1549	ASN
1	H	2045	GLN
1	H	2107	ASN
1	H	2140	HIS
1	H	2241	HIS
1	H	2267	GLN
1	H	2288	GLN
1	H	2316	GLN
1	H	2351	ASN
1	H	2372	GLN
1	H	2375	GLN
1	H	2528	GLN
1	H	2532	ASN
1	H	2534	GLN
1	H	2537	GLN
1	I	3140	HIS
1	I	3160	HIS
1	I	3184	HIS
1	I	3241	HIS
1	I	3316	GLN
1	I	3336	GLN
1	I	3351	ASN
1	I	3353	GLN
1	I	3375	GLN
1	I	3534	GLN
1	I	3537	GLN
1	I	3549	ASN
1	J	4045	GLN

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Mol	Chain	Res	Type
1	J	4079	ASN
1	J	4095	GLN
1	J	4107	ASN
1	J	4131	ASN
1	J	4140	HIS
1	J	4238	ASN
1	J	4241	HIS
1	J	4316	GLN
1	J	4336	GLN
1	J	4342	HIS
1	J	4351	ASN
1	J	4353	GLN
1	J	4375	GLN
1	J	4450	GLN
1	J	4537	GLN
1	K	5069	GLN
1	K	5131	ASN
1	K	5140	HIS
1	K	5160	HIS
1	K	5162	ASN
1	K	5241	HIS
1	K	5267	GLN
1	K	5288	GLN
1	K	5309	GLN
1	K	5336	GLN
1	K	5351	ASN
1	K	5353	GLN
1	K	5436	ASN
1	K	5437	HIS
1	K	5502	ASN
1	K	5522	GLN
1	K	5537	GLN
1	L	6107	ASN
1	L	6140	HIS
1	L	6238	ASN
1	L	6241	HIS
1	L	6351	ASN
1	L	6375	GLN
1	L	6450	GLN

### 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 ⓘ

25 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	NLX	A	1	-	26,29,29	3.43	16 (61%)	38,49,49	1.85	11 (28%)
2	NAG	A	179	-	14,14,15	0.62	0	15,19,21	0.74	0
2	NAG	A	180	-	14,14,15	0.58	0	15,19,21	0.74	1 (6%)
3	NLX	B	2	-	26,29,29	2.79	15 (57%)	38,49,49	1.74	9 (23%)
2	NAG	B	279	-	14,14,15	0.47	0	15,19,21	0.65	0
3	NLX	C	3	-	26,29,29	4.12	17 (65%)	38,49,49	5.43	15 (39%)
2	NAG	C	379	-	14,14,15	0.46	0	15,19,21	0.77	0
3	NLX	D	4	-	26,29,29	3.08	15 (57%)	38,49,49	1.91	13 (34%)
2	NAG	D	479	-	14,14,15	0.44	0	15,19,21	0.69	1 (6%)
3	NLX	E	5	-	26,29,29	2.89	15 (57%)	38,49,49	1.80	10 (26%)
2	NAG	E	579	-	14,14,15	0.49	0	15,19,21	0.83	1 (6%)
3	NLX	F	6	-	26,29,29	3.23	16 (61%)	38,49,49	5.35	17 (44%)
2	NAG	F	679	-	14,14,15	0.49	0	15,19,21	0.82	1 (6%)
3	NLX	G	1	-	26,29,29	3.18	15 (57%)	38,49,49	1.85	10 (26%)
2	NAG	G	179	-	14,14,15	0.55	0	15,19,21	0.67	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NLX	H	2	-	26,29,29	3.06	14 (53%)	38,49,49	1.98	11 (28%)
2	NAG	H	279	-	14,14,15	0.47	0	15,19,21	0.69	0
3	NLX	I	3	-	26,29,29	2.95	16 (61%)	38,49,49	1.93	11 (28%)
2	NAG	I	379	-	14,14,15	0.46	0	15,19,21	0.84	1 (6%)
3	NLX	J	4	-	26,29,29	3.18	14 (53%)	38,49,49	1.71	9 (23%)
2	NAG	J	479	-	14,14,15	0.54	0	15,19,21	0.71	1 (6%)
3	NLX	K	5	-	26,29,29	2.97	14 (53%)	38,49,49	1.76	10 (26%)
2	NAG	K	579	-	14,14,15	0.51	0	15,19,21	0.82	1 (6%)
3	NLX	L	6	-	26,29,29	3.15	15 (57%)	38,49,49	1.86	11 (28%)
2	NAG	L	679	-	14,14,15	0.59	0	15,19,21	0.72	1 (6%)

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	NLX	A	1	-	1/1/6/7	0/4/62/62	0/3/5/5
2	NAG	A	179	-	-	0/6/23/26	0/1/1/1
2	NAG	A	180	-	-	0/6/23/26	0/1/1/1
3	NLX	B	2	-	1/1/6/7	0/4/62/62	0/3/5/5
2	NAG	B	279	-	-	0/6/23/26	0/1/1/1
3	NLX	C	3	-	1/1/6/7	1/4/62/62	0/3/5/5
2	NAG	C	379	-	-	0/6/23/26	0/1/1/1
3	NLX	D	4	-	1/1/6/7	0/4/62/62	0/3/5/5
2	NAG	D	479	-	-	0/6/23/26	0/1/1/1
3	NLX	E	5	-	1/1/6/7	0/4/62/62	0/3/5/5
2	NAG	E	579	-	-	0/6/23/26	0/1/1/1
3	NLX	F	6	-	1/1/6/7	0/4/62/62	0/3/5/5
2	NAG	F	679	-	-	0/6/23/26	0/1/1/1
3	NLX	G	1	-	1/1/6/7	0/4/62/62	0/3/5/5
2	NAG	G	179	-	-	0/6/23/26	0/1/1/1
3	NLX	H	2	-	1/1/6/7	0/4/62/62	0/3/5/5
2	NAG	H	279	-	-	0/6/23/26	0/1/1/1
3	NLX	I	3	-	1/1/6/7	0/4/62/62	0/3/5/5
2	NAG	I	379	-	-	0/6/23/26	0/1/1/1
3	NLX	J	4	-	1/1/6/7	0/4/62/62	0/3/5/5
2	NAG	J	479	-	-	0/6/23/26	0/1/1/1
3	NLX	K	5	-	1/1/6/7	0/4/62/62	0/3/5/5
2	NAG	K	579	-	-	0/6/23/26	0/1/1/1
3	NLX	L	6	-	1/1/6/7	0/4/62/62	0/3/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	L	679	-	-	0/6/23/26	0/1/1/1

All (182) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	4	NLX	C13-C12	2.01	1.54	1.50
3	K	5	NLX	C1-C11	2.03	1.43	1.39
3	E	5	NLX	C13-C12	2.05	1.54	1.50
3	K	5	NLX	C2-C3	2.05	1.43	1.39
3	G	1	NLX	C2-C3	2.05	1.43	1.39
3	D	4	NLX	C13-C12	2.06	1.54	1.50
3	D	4	NLX	C3-C4	2.06	1.44	1.40
3	I	3	NLX	C2-C3	2.08	1.43	1.39
3	F	6	NLX	C16-N1	2.09	1.57	1.52
3	A	1	NLX	C3-C4	2.09	1.44	1.40
3	H	2	NLX	C4-C12	2.09	1.41	1.38
3	K	5	NLX	C5-C6	2.13	1.58	1.52
3	D	4	NLX	O2-C5	2.13	1.50	1.47
3	G	1	NLX	C8-C7	2.15	1.57	1.53
3	A	1	NLX	C13-C12	2.16	1.54	1.50
3	F	6	NLX	C19-C18	2.16	1.43	1.28
3	C	3	NLX	C16-C15	2.19	1.56	1.52
3	A	1	NLX	C5-C6	2.20	1.59	1.52
3	I	3	NLX	C2-C1	2.21	1.42	1.38
3	C	3	NLX	C2-C3	2.21	1.43	1.39
3	J	4	NLX	O2-C5	2.22	1.50	1.47
3	I	3	NLX	C4-C12	2.25	1.41	1.38
3	I	3	NLX	O2-C5	2.27	1.50	1.47
3	A	1	NLX	O2-C5	2.29	1.50	1.47
3	H	2	NLX	C3-C4	2.30	1.45	1.40
3	J	4	NLX	C2-C1	2.32	1.42	1.38
3	L	6	NLX	C3-C4	2.33	1.45	1.40
3	B	2	NLX	C2-C3	2.34	1.43	1.39
3	I	3	NLX	C5-C6	2.36	1.59	1.52
3	B	2	NLX	C5-C6	2.37	1.59	1.52
3	B	2	NLX	C7-C6	2.38	1.54	1.50
3	F	6	NLX	C10-C11	2.39	1.55	1.51
3	L	6	NLX	C13-C12	2.40	1.54	1.50
3	E	5	NLX	C3-C4	2.40	1.45	1.40
3	A	1	NLX	C8-C7	2.41	1.58	1.53
3	D	4	NLX	C2-C1	2.41	1.43	1.38
3	H	2	NLX	C13-C12	2.42	1.54	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	1	NLX	O2-C5	2.42	1.50	1.47
3	E	5	NLX	C5-C6	2.46	1.59	1.52
3	D	4	NLX	C4-C12	2.47	1.42	1.38
3	C	3	NLX	O2-C4	2.48	1.42	1.38
3	C	3	NLX	C15-C13	2.48	1.57	1.54
3	D	4	NLX	C16-C15	2.48	1.57	1.52
3	L	6	NLX	C5-C6	2.49	1.59	1.52
3	B	2	NLX	C4-C12	2.52	1.42	1.38
3	H	2	NLX	C16-C15	2.55	1.57	1.52
3	D	4	NLX	C8-C7	2.55	1.58	1.53
3	I	3	NLX	C10-C11	2.60	1.56	1.51
3	K	5	NLX	C13-C5	2.63	1.58	1.54
3	A	1	NLX	C2-C1	2.66	1.43	1.38
3	G	1	NLX	C5-C6	2.66	1.60	1.52
3	L	6	NLX	C2-C1	2.66	1.43	1.38
3	G	1	NLX	C4-C12	2.67	1.42	1.38
3	I	3	NLX	C3-C4	2.69	1.45	1.40
3	C	3	NLX	C2-C1	2.72	1.43	1.38
3	G	1	NLX	C2-C1	2.72	1.43	1.38
3	E	5	NLX	C4-C12	2.72	1.42	1.38
3	B	2	NLX	C2-C1	2.76	1.43	1.38
3	E	5	NLX	C2-C1	2.77	1.43	1.38
3	I	3	NLX	C8-C14	2.78	1.57	1.53
3	J	4	NLX	C8-C7	2.78	1.59	1.53
3	L	6	NLX	O2-C5	2.79	1.51	1.47
3	K	5	NLX	C4-C12	2.79	1.42	1.38
3	H	2	NLX	C8-C7	2.81	1.59	1.53
3	H	2	NLX	C10-C11	2.82	1.56	1.51
3	F	6	NLX	C8-C14	2.82	1.57	1.53
3	E	5	NLX	C13-C5	2.82	1.58	1.54
3	H	2	NLX	O2-C5	2.84	1.51	1.47
3	B	2	NLX	C13-C5	2.85	1.58	1.54
3	I	3	NLX	C7-C6	2.86	1.55	1.50
3	B	2	NLX	C13-C12	2.90	1.55	1.50
3	E	5	NLX	C8-C14	2.91	1.57	1.53
3	B	2	NLX	O2-C5	2.92	1.51	1.47
3	E	5	NLX	C7-C6	2.93	1.55	1.50
3	E	5	NLX	O2-C5	2.94	1.51	1.47
3	L	6	NLX	C11-C12	2.95	1.44	1.39
3	J	4	NLX	C4-C12	2.96	1.42	1.38
3	I	3	NLX	C16-C15	2.97	1.58	1.52
3	L	6	NLX	C4-C12	2.99	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	5	NLX	C11-C12	3.02	1.44	1.39
3	J	4	NLX	C10-C11	3.03	1.56	1.51
3	C	3	NLX	C3-C4	3.05	1.46	1.40
3	A	1	NLX	C4-C12	3.12	1.43	1.38
3	C	3	NLX	C7-C6	3.12	1.56	1.50
3	D	4	NLX	C13-C5	3.14	1.58	1.54
3	E	5	NLX	C16-C15	3.14	1.58	1.52
3	K	5	NLX	C2-C1	3.14	1.44	1.38
3	C	3	NLX	C8-C7	3.18	1.60	1.53
3	K	5	NLX	C16-C15	3.18	1.58	1.52
3	D	4	NLX	C7-C6	3.19	1.56	1.50
3	L	6	NLX	C13-C5	3.21	1.59	1.54
3	I	3	NLX	C13-C12	3.22	1.56	1.50
3	B	2	NLX	C8-C14	3.22	1.58	1.53
3	H	2	NLX	C7-C6	3.23	1.56	1.50
3	F	6	NLX	C13-C5	3.23	1.59	1.54
3	B	2	NLX	C16-C15	3.24	1.58	1.52
3	I	3	NLX	C13-C5	3.27	1.59	1.54
3	F	6	NLX	C13-C12	3.42	1.56	1.50
3	L	6	NLX	C16-C15	3.47	1.59	1.52
3	F	6	NLX	C7-C6	3.51	1.56	1.50
3	B	2	NLX	C10-C11	3.53	1.57	1.51
3	H	2	NLX	C13-C5	3.53	1.59	1.54
3	J	4	NLX	C16-C15	3.53	1.59	1.52
3	F	6	NLX	C20-N1	3.53	1.61	1.50
3	C	3	NLX	C4-C12	3.54	1.43	1.38
3	K	5	NLX	C8-C14	3.54	1.58	1.53
3	K	5	NLX	C11-C12	3.56	1.45	1.39
3	H	2	NLX	C8-C14	3.60	1.58	1.53
3	L	6	NLX	C7-C6	3.61	1.56	1.50
3	G	1	NLX	C16-C15	3.62	1.59	1.52
3	F	6	NLX	C2-C3	3.64	1.46	1.39
3	C	3	NLX	C13-C12	3.64	1.56	1.50
3	D	4	NLX	C8-C14	3.65	1.58	1.53
3	G	1	NLX	C7-C6	3.67	1.57	1.50
3	A	1	NLX	C11-C12	3.67	1.45	1.39
3	J	4	NLX	C7-C6	3.68	1.57	1.50
3	F	6	NLX	C17-C18	3.71	1.63	1.50
3	K	5	NLX	C7-C6	3.71	1.57	1.50
3	G	1	NLX	C11-C12	3.72	1.45	1.39
3	I	3	NLX	C11-C12	3.73	1.45	1.39
3	G	1	NLX	C13-C5	3.74	1.59	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1	NLX	C10-C11	3.80	1.58	1.51
3	H	2	NLX	C11-C12	3.81	1.45	1.39
3	D	4	NLX	C10-C11	3.82	1.58	1.51
3	J	4	NLX	C11-C12	3.91	1.45	1.39
3	A	1	NLX	C7-C6	3.91	1.57	1.50
3	F	6	NLX	C16-C15	3.96	1.60	1.52
3	F	6	NLX	O2-C5	4.04	1.53	1.47
3	L	6	NLX	C8-C14	4.07	1.59	1.53
3	B	2	NLX	C11-C12	4.10	1.46	1.39
3	F	6	NLX	C8-C7	4.10	1.62	1.53
3	G	1	NLX	C10-C11	4.17	1.58	1.51
3	D	4	NLX	C15-C13	4.17	1.60	1.54
3	E	5	NLX	C15-C13	4.22	1.60	1.54
3	J	4	NLX	C15-C13	4.23	1.60	1.54
3	A	1	NLX	C16-C15	4.26	1.60	1.52
3	H	2	NLX	C15-C13	4.30	1.60	1.54
3	D	4	NLX	C11-C12	4.34	1.46	1.39
3	K	5	NLX	C15-C13	4.34	1.60	1.54
3	E	5	NLX	C10-C11	4.34	1.59	1.51
3	L	6	NLX	C10-C11	4.35	1.59	1.51
3	K	5	NLX	C10-C11	4.36	1.59	1.51
3	A	1	NLX	C13-C5	4.40	1.60	1.54
3	J	4	NLX	C8-C14	4.41	1.60	1.53
3	J	4	NLX	C13-C5	4.41	1.60	1.54
3	B	2	NLX	C15-C13	4.47	1.60	1.54
3	I	3	NLX	C15-C13	4.49	1.60	1.54
3	C	3	NLX	C8-C14	4.62	1.60	1.53
3	A	1	NLX	C8-C14	4.71	1.60	1.53
3	C	3	NLX	O2-C5	4.78	1.54	1.47
3	F	6	NLX	C14-C9	4.82	1.63	1.55
3	C	3	NLX	C13-C5	4.87	1.61	1.54
3	G	1	NLX	C8-C14	4.87	1.60	1.53
3	G	1	NLX	C15-C13	4.92	1.61	1.54
3	L	6	NLX	C15-C13	5.07	1.61	1.54
3	D	4	NLX	C14-C13	5.14	1.61	1.53
3	C	3	NLX	C11-C12	5.27	1.48	1.39
3	A	1	NLX	C15-C13	5.40	1.62	1.54
3	E	5	NLX	C14-C13	5.43	1.61	1.53
3	J	4	NLX	C14-C13	5.69	1.62	1.53
3	H	2	NLX	C14-C13	5.75	1.62	1.53
3	C	3	NLX	C14-C13	5.75	1.62	1.53
3	B	2	NLX	C14-C9	5.78	1.65	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2	NLX	C14-C13	5.79	1.62	1.53
3	K	5	NLX	C14-C13	5.88	1.62	1.53
3	I	3	NLX	C14-C13	5.89	1.62	1.53
3	C	3	NLX	C10-C11	5.98	1.62	1.51
3	G	1	NLX	C14-C13	6.08	1.62	1.53
3	L	6	NLX	C14-C13	6.23	1.63	1.53
3	F	6	NLX	C14-C13	6.27	1.63	1.53
3	A	1	NLX	C14-C13	6.61	1.63	1.53
3	F	6	NLX	C11-C12	6.87	1.50	1.39
3	E	5	NLX	C14-C9	7.22	1.67	1.55
3	K	5	NLX	C14-C9	7.32	1.68	1.55
3	G	1	NLX	C14-C9	7.54	1.68	1.55
3	L	6	NLX	C14-C9	7.67	1.68	1.55
3	I	3	NLX	C14-C9	7.87	1.69	1.55
3	A	1	NLX	C14-C9	8.62	1.70	1.55
3	J	4	NLX	C14-C9	8.72	1.70	1.55
3	H	2	NLX	C14-C9	9.04	1.71	1.55
3	D	4	NLX	C14-C9	9.26	1.71	1.55
3	C	3	NLX	C14-C9	13.31	1.78	1.55

All (145) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	3	NLX	C20-N1-C17	-24.38	63.74	108.74
3	F	6	NLX	C20-N1-C17	-23.08	66.14	108.74
3	C	3	NLX	C20-N1-C16	-17.31	68.71	108.68
3	F	6	NLX	C20-N1-C16	-15.98	71.79	108.68
3	H	2	NLX	C8-C14-C13	-4.32	107.38	111.33
3	C	3	NLX	C8-C14-C13	-4.27	107.42	111.33
3	C	3	NLX	C16-N1-C9	-3.92	98.54	108.99
3	F	6	NLX	C15-C13-C12	-3.79	103.26	111.72
3	A	1	NLX	C20-N1-C17	-3.73	101.85	108.74
3	D	4	NLX	C8-C14-C13	-3.69	107.95	111.33
3	J	4	NLX	C8-C14-C13	-3.47	108.15	111.33
3	L	6	NLX	C20-N1-C17	-3.44	102.39	108.74
3	F	6	NLX	C17-N1-C9	-3.36	104.68	110.41
3	B	2	NLX	O3-C6-C7	-3.35	116.38	122.08
3	A	1	NLX	C8-C14-C13	-3.32	108.29	111.33
3	I	3	NLX	C8-C14-C13	-3.31	108.30	111.33
3	J	4	NLX	C20-N1-C17	-3.29	102.67	108.74
3	F	6	NLX	C14-C13-C12	-2.96	104.02	108.36
3	E	5	NLX	O3-C6-C7	-2.93	117.09	122.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	5	NLX	C20-N1-C17	-2.91	103.36	108.74
3	C	3	NLX	C17-N1-C9	-2.91	105.45	110.41
3	E	5	NLX	C8-C14-C13	-2.87	108.70	111.33
3	G	1	NLX	O3-C6-C7	-2.78	117.35	122.08
3	L	6	NLX	O2-C4-C12	-2.74	109.30	112.86
3	I	3	NLX	O3-C6-C7	-2.71	117.47	122.08
3	L	6	NLX	O3-C6-C7	-2.70	117.48	122.08
3	F	6	NLX	O4-C14-C8	-2.70	102.28	107.97
3	G	1	NLX	C20-N1-C17	-2.67	103.81	108.74
2	I	379	NAG	C2-N2-C7	-2.66	119.63	123.04
3	B	2	NLX	C20-N1-C17	-2.66	103.84	108.74
3	C	3	NLX	O2-C4-C12	-2.63	109.44	112.86
3	E	5	NLX	O2-C4-C12	-2.62	109.45	112.86
3	H	2	NLX	C20-N1-C17	-2.61	103.93	108.74
3	I	3	NLX	C20-N1-C17	-2.59	103.95	108.74
3	F	6	NLX	C12-C13-C5	-2.59	95.56	98.61
2	K	579	NAG	C2-N2-C7	-2.57	119.74	123.04
2	F	679	NAG	C2-N2-C7	-2.54	119.78	123.04
2	E	579	NAG	C2-N2-C7	-2.52	119.80	123.04
3	I	3	NLX	O2-C4-C12	-2.50	109.60	112.86
3	D	4	NLX	C20-N1-C9	-2.50	107.71	112.84
3	L	6	NLX	C8-C14-C13	-2.49	109.04	111.33
3	D	4	NLX	C20-N1-C17	-2.48	104.16	108.74
3	K	5	NLX	O3-C6-C7	-2.46	117.89	122.08
3	K	5	NLX	C20-N1-C17	-2.41	104.30	108.74
3	F	6	NLX	C8-C14-C13	-2.40	109.13	111.33
3	K	5	NLX	O2-C4-C12	-2.39	109.75	112.86
3	A	1	NLX	O3-C6-C7	-2.39	118.02	122.08
3	G	1	NLX	C15-C13-C12	-2.38	106.40	111.72
3	F	6	NLX	C3-C4-C12	-2.37	117.71	120.89
3	H	2	NLX	O2-C4-C12	-2.35	109.80	112.86
3	B	2	NLX	O2-C4-C12	-2.30	109.86	112.86
3	A	1	NLX	O2-C4-C12	-2.30	109.86	112.86
3	H	2	NLX	C20-N1-C9	-2.29	108.14	112.84
3	D	4	NLX	O2-C4-C12	-2.29	109.88	112.86
3	B	2	NLX	C8-C14-C13	-2.24	109.28	111.33
3	K	5	NLX	C8-C14-C13	-2.23	109.28	111.33
3	G	1	NLX	O2-C4-C12	-2.21	109.98	112.86
3	D	4	NLX	O3-C6-C7	-2.15	118.41	122.08
3	A	1	NLX	C12-C13-C5	-2.14	96.09	98.61
2	J	479	NAG	C2-N2-C7	-2.13	120.30	123.04
2	D	479	NAG	C2-N2-C7	-2.13	120.31	123.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	3	NLX	C12-C13-C5	-2.13	96.10	98.61
3	C	3	NLX	C15-C13-C14	-2.10	107.24	109.32
2	L	679	NAG	C2-N2-C7	-2.09	120.36	123.04
2	A	180	NAG	C2-N2-C7	-2.08	120.37	123.04
3	H	2	NLX	O3-C6-C7	-2.06	118.57	122.08
3	C	3	NLX	C3-C4-C12	-2.03	118.17	120.89
3	J	4	NLX	O3-C6-C7	-2.02	118.64	122.08
3	L	6	NLX	C12-C13-C5	-2.01	96.24	98.61
3	D	4	NLX	C13-C12-C4	2.15	111.44	109.34
3	J	4	NLX	C17-N1-C9	2.16	114.08	110.41
3	I	3	NLX	C17-N1-C9	2.17	114.10	110.41
3	A	1	NLX	C17-N1-C9	2.19	114.14	110.41
3	L	6	NLX	C15-C13-C14	2.21	111.50	109.32
3	D	4	NLX	C15-C13-C14	2.25	111.54	109.32
3	F	6	NLX	C16-N1-C9	2.28	115.06	108.99
3	G	1	NLX	C15-C13-C14	2.28	111.57	109.32
3	K	5	NLX	C13-C12-C4	2.28	111.57	109.34
3	B	2	NLX	C13-C12-C4	2.28	111.57	109.34
3	G	1	NLX	C13-C12-C4	2.35	111.63	109.34
3	D	4	NLX	C4-O2-C5	2.35	107.29	104.80
3	F	6	NLX	C16-C15-C13	2.36	115.58	111.54
3	C	3	NLX	C15-C13-C5	2.42	114.87	111.77
3	F	6	NLX	C7-C6-C5	2.42	120.81	116.35
3	J	4	NLX	C13-C12-C4	2.44	111.72	109.34
3	E	5	NLX	C17-N1-C9	2.47	114.62	110.41
3	K	5	NLX	O2-C4-C3	2.53	130.68	126.09
3	I	3	NLX	C13-C12-C4	2.60	111.88	109.34
3	C	3	NLX	C16-C15-C13	2.60	115.98	111.54
3	K	5	NLX	C15-C13-C14	2.61	111.90	109.32
3	E	5	NLX	C13-C12-C4	2.64	111.92	109.34
3	J	4	NLX	O2-C4-C3	2.65	130.91	126.09
3	C	3	NLX	C7-C6-C5	2.67	121.27	116.35
3	J	4	NLX	O2-C5-C6	2.69	111.43	108.37
3	B	2	NLX	O2-C4-C3	2.73	131.06	126.09
3	H	2	NLX	C13-C12-C4	2.74	112.02	109.34
3	D	4	NLX	O2-C4-C3	2.75	131.10	126.09
3	G	1	NLX	O2-C4-C3	2.76	131.11	126.09
3	A	1	NLX	O2-C4-C3	2.78	131.15	126.09
3	L	6	NLX	O2-C4-C3	2.80	131.19	126.09
3	I	3	NLX	O2-C4-C3	2.85	131.28	126.09
3	E	5	NLX	O2-C4-C3	2.87	131.31	126.09
3	L	6	NLX	C13-C12-C4	2.88	112.16	109.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	6	NLX	C13-C12-C4	2.90	112.17	109.34
3	A	1	NLX	C13-C12-C4	2.94	112.21	109.34
3	H	2	NLX	O2-C4-C3	3.06	131.66	126.09
3	B	2	NLX	C16-C15-C13	3.12	116.87	111.54
3	H	2	NLX	C7-C6-C5	3.14	122.14	116.35
3	F	6	NLX	O2-C4-C3	3.17	131.85	126.09
3	D	4	NLX	C7-C6-C5	3.25	122.34	116.35
3	I	3	NLX	C7-C6-C5	3.27	122.37	116.35
3	C	3	NLX	C13-C12-C4	3.30	112.57	109.34
3	J	4	NLX	C7-C6-C5	3.35	122.53	116.35
3	E	5	NLX	C16-C15-C13	3.41	117.37	111.54
3	C	3	NLX	O2-C4-C3	3.45	132.36	126.09
3	B	2	NLX	C7-C6-C5	3.51	122.82	116.35
3	A	1	NLX	C7-C6-C5	3.53	122.85	116.35
3	K	5	NLX	C16-C15-C13	3.54	117.59	111.54
3	L	6	NLX	C16-C15-C13	3.55	117.61	111.54
3	E	5	NLX	C7-C6-C5	3.59	122.97	116.35
3	K	5	NLX	C7-C6-C5	3.63	123.03	116.35
3	G	1	NLX	C16-C15-C13	3.71	117.87	111.54
3	G	1	NLX	C7-C6-C5	3.72	123.21	116.35
3	D	4	NLX	O2-C5-C6	3.73	112.62	108.37
3	L	6	NLX	C7-C6-C5	3.79	123.33	116.35
3	A	1	NLX	O2-C5-C6	3.84	112.74	108.37
3	C	3	NLX	O2-C5-C6	3.88	112.80	108.37
3	D	4	NLX	C16-C15-C13	3.94	118.27	111.54
3	A	1	NLX	C16-C15-C13	3.95	118.29	111.54
3	H	2	NLX	C16-C15-C13	3.96	118.30	111.54
3	I	3	NLX	C16-C15-C13	3.97	118.32	111.54
3	H	2	NLX	C17-N1-C9	4.20	117.56	110.41
3	J	4	NLX	C16-C15-C13	4.22	118.74	111.54
3	D	4	NLX	C17-N1-C9	4.33	117.77	110.41
3	H	2	NLX	O2-C5-C6	4.39	113.38	108.37
3	E	5	NLX	O2-C5-C6	4.39	113.38	108.37
3	L	6	NLX	O2-C5-C6	4.85	113.90	108.37
3	K	5	NLX	O2-C5-C6	4.86	113.91	108.37
3	B	2	NLX	O2-C5-C6	5.02	114.09	108.37
3	I	3	NLX	O2-C5-C6	5.55	114.70	108.37
3	G	1	NLX	O2-C5-C6	5.76	114.94	108.37
3	F	6	NLX	C15-C13-C14	7.17	116.41	109.32
3	F	6	NLX	O2-C5-C6	7.48	116.90	108.37
3	F	6	NLX	C16-N1-C17	8.51	129.74	109.03
3	C	3	NLX	C16-N1-C17	9.33	131.74	109.03

All (12) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	C	3	NLX	N1
3	K	5	NLX	N1
3	L	6	NLX	N1
3	J	4	NLX	N1
3	F	6	NLX	N1
3	H	2	NLX	N1
3	E	5	NLX	N1
3	D	4	NLX	N1
3	B	2	NLX	N1
3	G	1	NLX	N1
3	A	1	NLX	N1
3	I	3	NLX	N1

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	3	NLX	C19-C18-C17-N1

There are no ring outliers.

22 monomers are involved in 273 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1	NLX	20	0
2	A	179	NAG	3	0
2	A	180	NAG	1	0
3	B	2	NLX	21	0
2	B	279	NAG	4	0
3	C	3	NLX	27	0
3	D	4	NLX	15	0
2	D	479	NAG	4	0
3	E	5	NLX	18	0
2	E	579	NAG	2	0
3	F	6	NLX	23	0
3	G	1	NLX	12	0
2	G	179	NAG	4	0
3	H	2	NLX	30	0
2	H	279	NAG	1	0
3	I	3	NLX	19	0
2	I	379	NAG	1	0
3	J	4	NLX	20	0
2	J	479	NAG	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	K	5	NLX	18	0
2	K	579	NAG	1	0
3	L	6	NLX	23	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.



## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.