



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 02:59 AM UTC

PDB ID : 1MX9 / pdb_00001mx9
Title : Crystal Structure of Human Liver Carboxylesterase in complexed with nalox-one 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

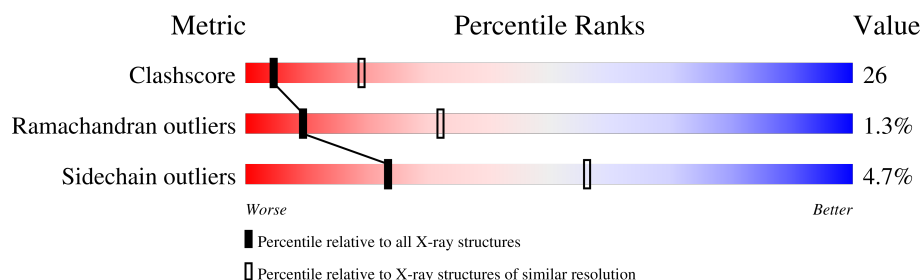
1 Overall quality at a glance

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	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	548	51% 42% . .
1	B	548	59% 34% . .
1	C	548	57% 36% . .
1	D	548	60% 34% . .
1	E	548	54% 38% 5% .
1	F	548	53% 41% . .
1	G	548	51% 41% 5% .
1	H	548	55% 38% . .

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Mol	Chain	Length	Quality of chain
1	I	548	 49% 44% 5% .
1	J	548	 53% 41% . .
1	K	548	 51% 41% . .
1	L	548	 51% 41% 5% .

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:

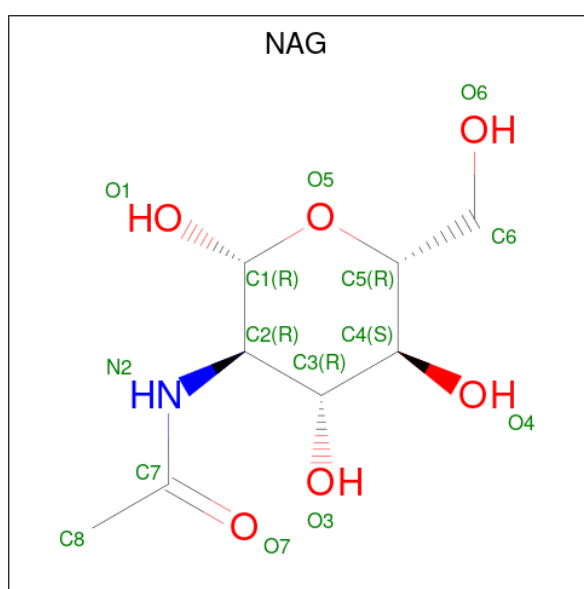
Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	GLN	deletion	UNP P23141
B	?	-	GLN	deletion	UNP P23141
C	?	-	GLN	deletion	UNP P23141
D	?	-	GLN	deletion	UNP P23141
E	?	-	GLN	deletion	UNP P23141

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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 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



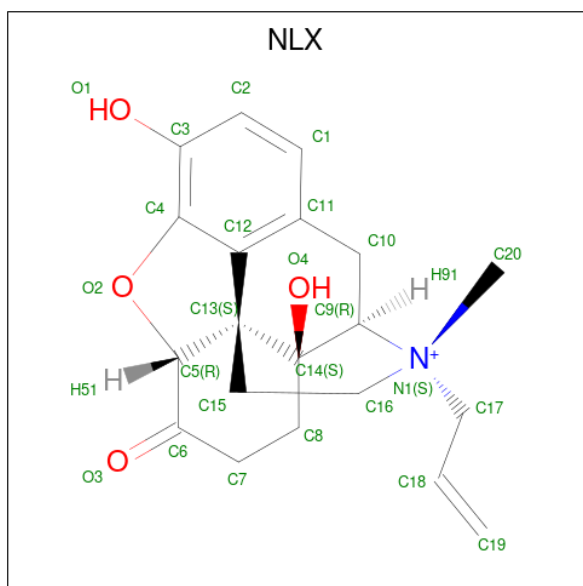
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	E	1	Total	C	N	O	0	0
			14	8	1	5		
2	F	1	Total	C	N	O	0	0
			14	8	1	5		

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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 (CCD ID: NLX) (formula: C₂₀H₂₄NO₄).



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.

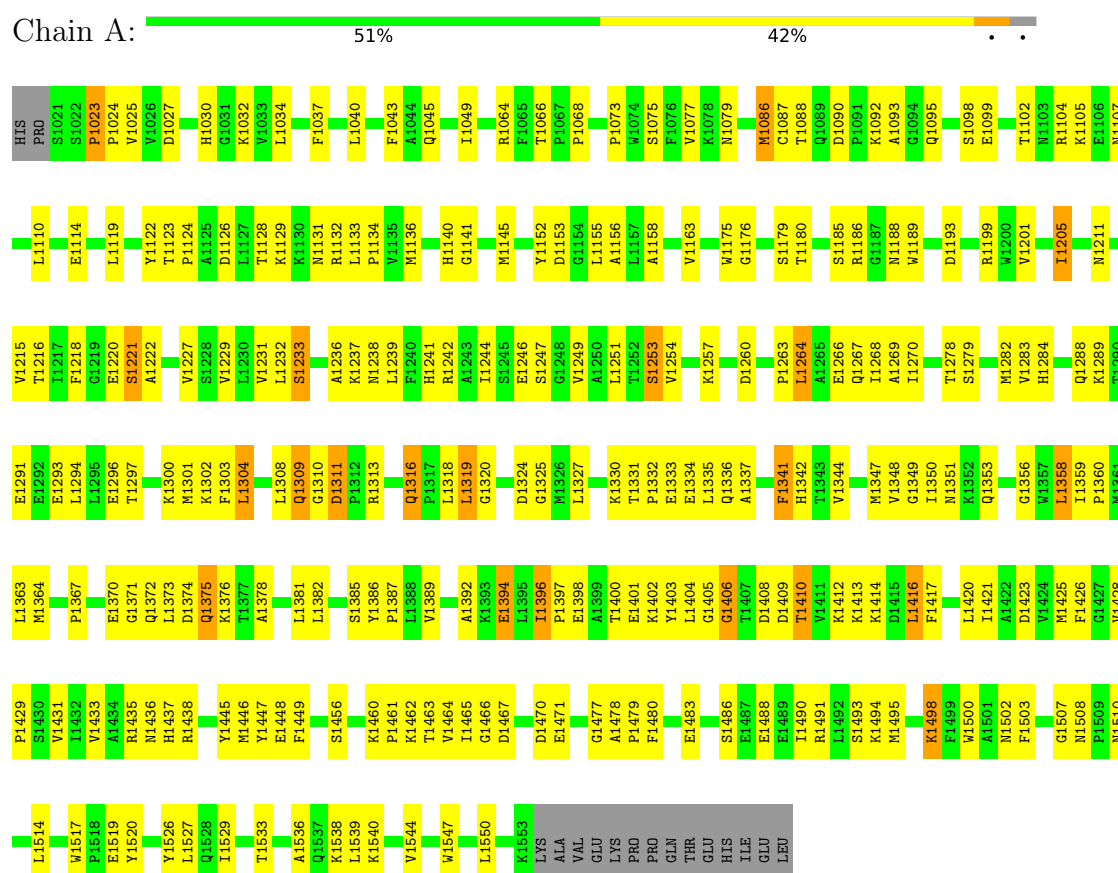
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	87	Total	O	0	0
			87	87		
4	B	120	Total	O	0	0
			120	120		
4	C	98	Total	O	0	0
			98	98		
4	D	119	Total	O	0	0
			119	119		
4	E	112	Total	O	0	0
			112	112		
4	F	91	Total	O	0	0
			91	91		
4	G	69	Total	O	0	0
			69	69		
4	H	95	Total	O	0	0
			95	95		
4	I	80	Total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

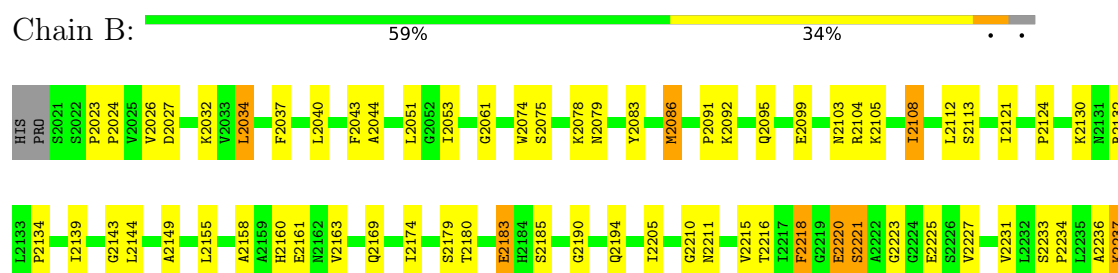
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

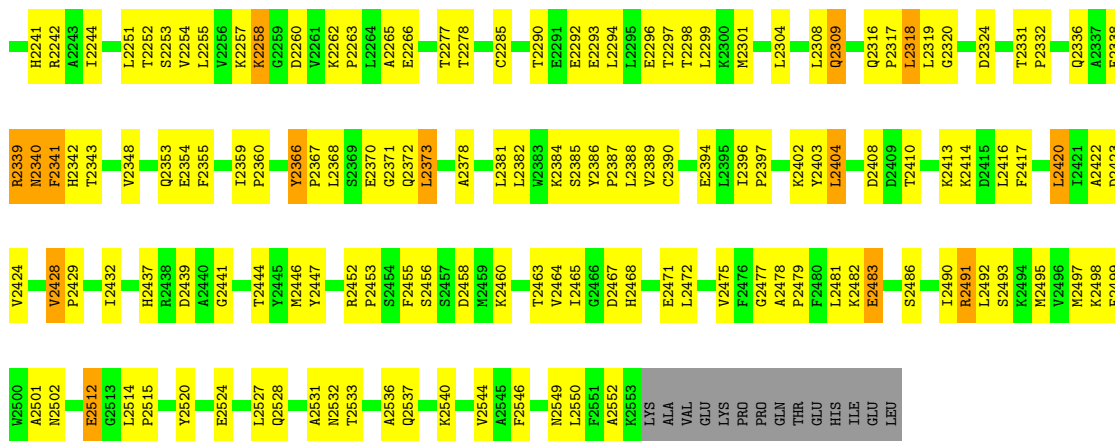
Note EDS was not executed.

- Molecule 1: liver Carboxylesterase I



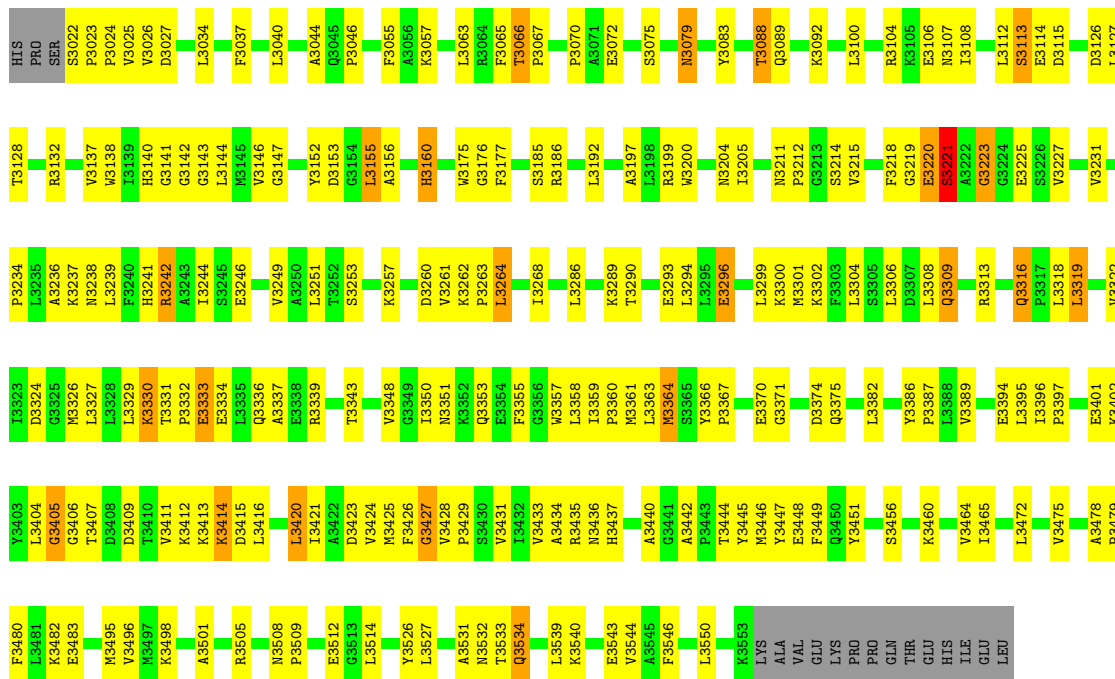
- Molecule 1: liver Carboxylesterase I





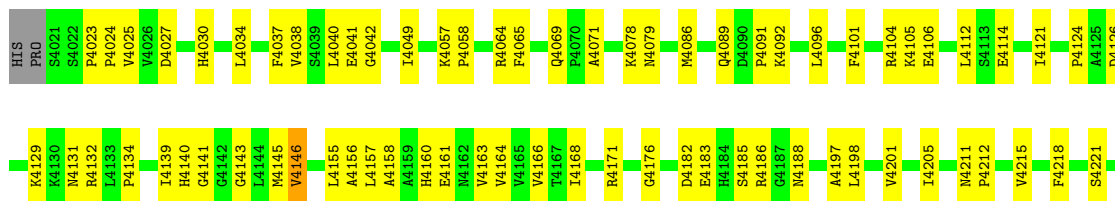
• Molecule 1: liver Carboxylesterase I

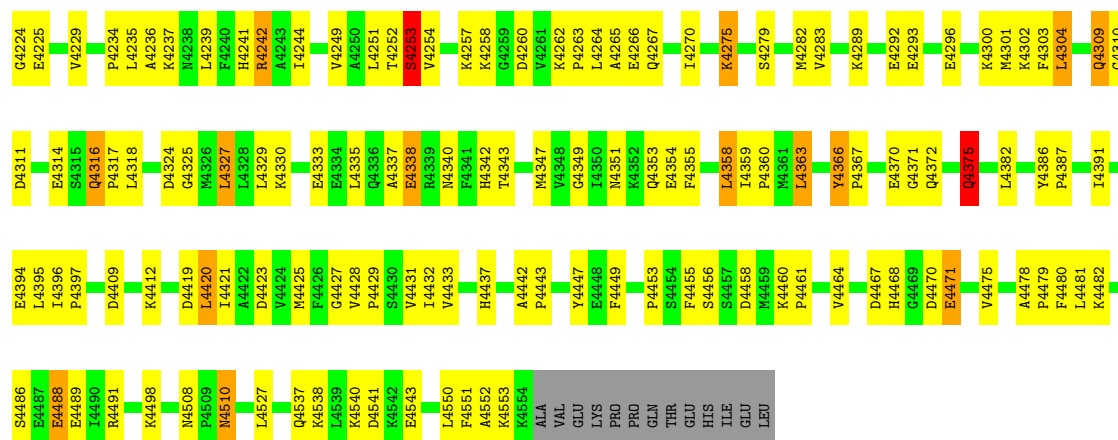
Chain C: 57% 36%



• Molecule 1: liver Carboxylesterase I

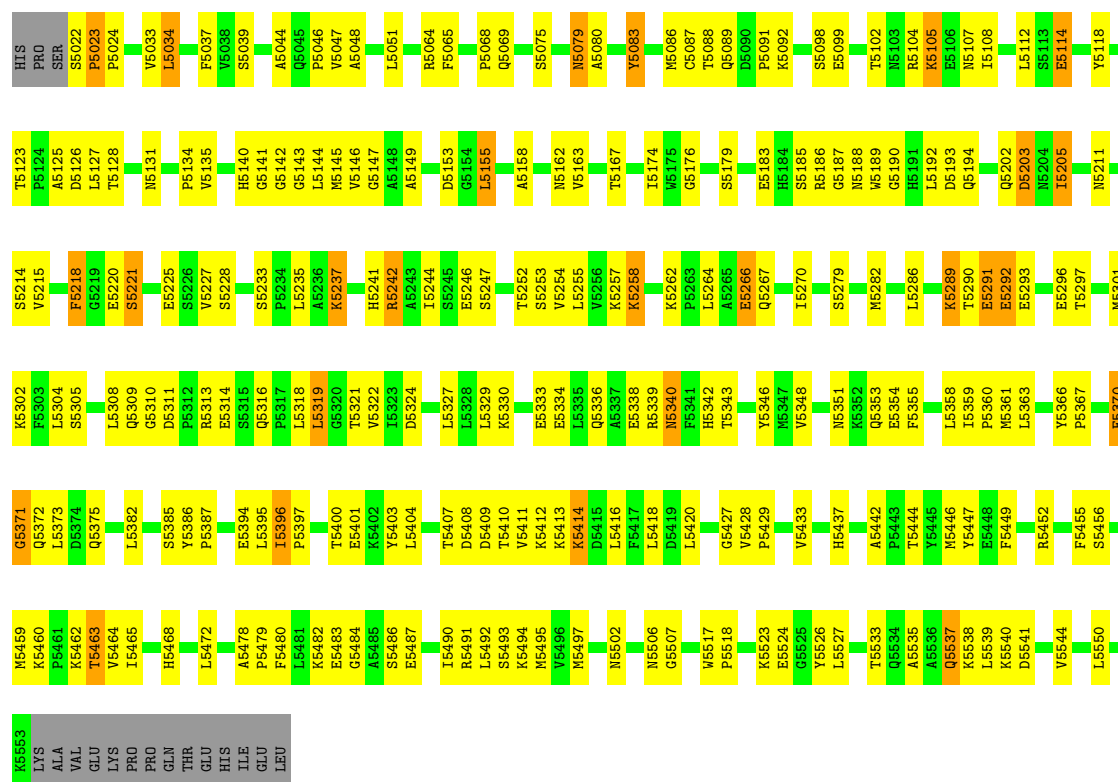
Chain D: 60% 34%





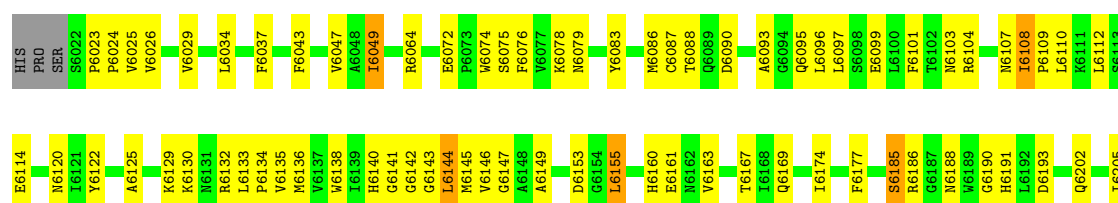
• Molecule 1: liver Carboxylesterase I

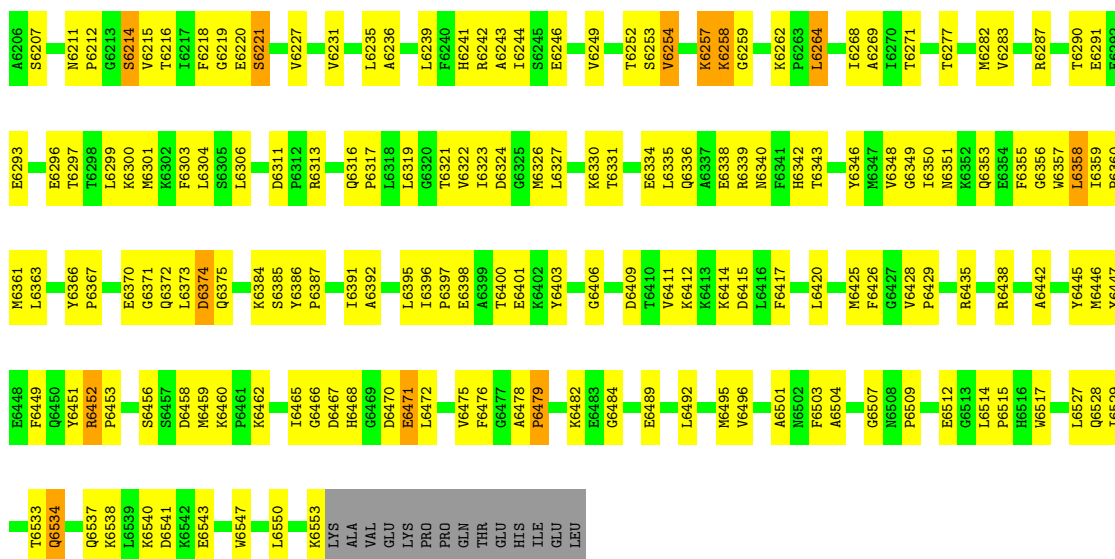
Chain E: 54% 38% 5% •



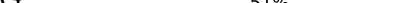
• Molecule 1: liver Carboxylesterase I

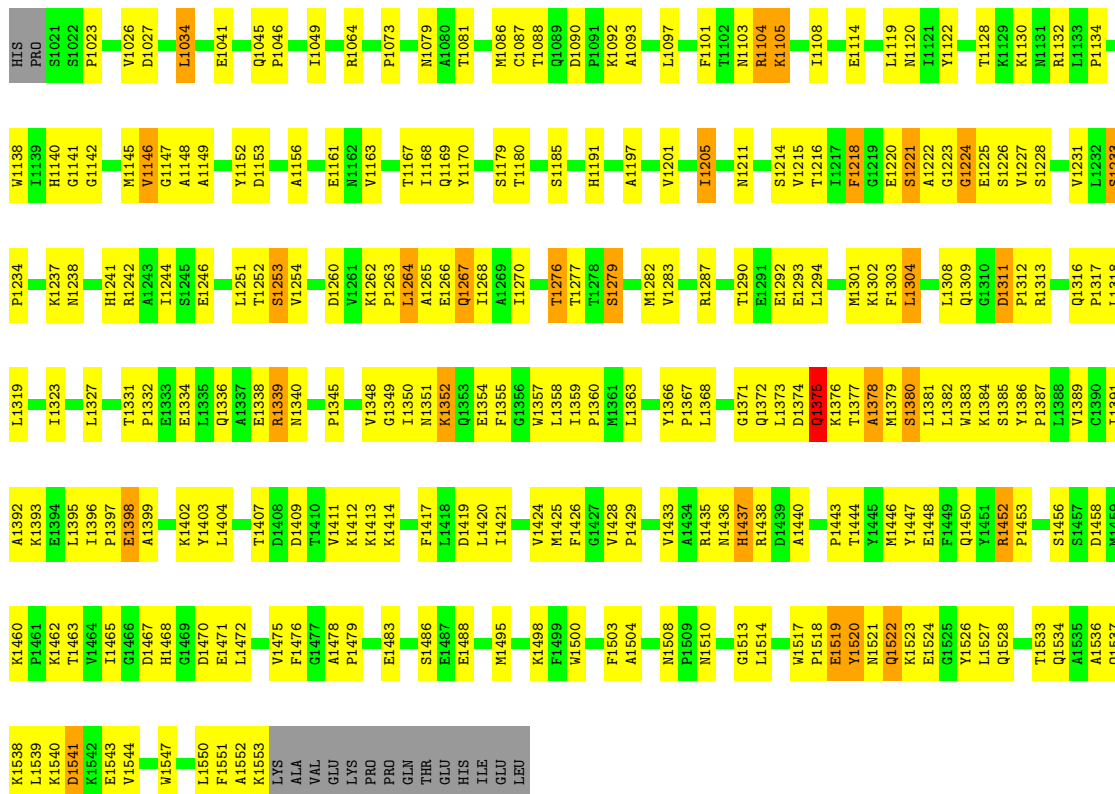
Chain F: 53% 41% • •



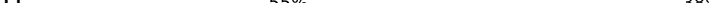


- Molecule 1: liver Carboxylesterase I

Chain G:  51% 41% 5%

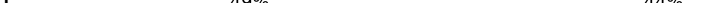


- Molecule 1: liver Carboxylesterase I

Chain H:  55% 38% 7%

K2553	LYS	M2459	Q2372	L2299	V2215	S2113
	K2460	L2373	K2300	M2301	T2216	E2114
	ALA	D2374	M2302			
	VAL	K2462	Q2375	K2302	L2119	
	GLU	T2463	K2376	F2303	M2120	
	LYS	T2464		E2220	L2121	
	PRO	T2465	M2379	L2304	S2221	
	PRO	G2466		S2305	A2222	
	GLN	D2467	L2382	L2306	T2123	
	THR	H2468				
K2554	GLU	G2469	S2386	Q2309	G2224	D2126
	D2470	Y2386	G2310	E2225	L2127	K2032
	HIS	P2387	D2311	S2226	T2128	W2033
	ILE	E2471	P2387	F2312	K2129	L2034
	LEU	L2472	L2388	M2313		G2035
			V2389	E2314		K2036
				S2315	R2132	F2037
		A2478	I2396	G2316	L2133	
		T2479	P2397	L2317	P2134	
		F2480		L2318		L2040
K2555	GLN	L2481	T2400	L2319	A2236	E2041
		E2483	E2401	K2237	N2238	
		S2486	K2402	D2324	H2241	A2048
			Y2403	L2327	R2242	K2057
			L2404		G2142	
				K2330	G2143	
		T2490	D2409		L2144	
		R2491	T2410	E2334	M2145	
		L2492	Y2411		Y2152	G2061
						R2064
K2556	GLU	V2496	K2412	E2338	L2155	
		N2497	K2413	R2339	T2252	E2072
		K2498	K2414	M2340	S2253	F2073
		T2499		F2341	T2254	W2074
		W2500	F2417	L2255	V2163	
		A2501		H2342	V2164	K2078
		N2502	L2420	T2343	V2256	N2079
				K2257	V2166	A2080
				V2344	K2258	T2081
		R2505	D2423	F2345	G2259	S2082
K2557			V2424	Y2346	D2260	Y2083
	L2514	M2425	M2347	M2347		
		F2426	V2348	L2264	G2176	
	E2524	G2427	G2349	T2264	F2177	K2086
	G2525	V2428	L2350	A2265	F2178	C2087
	Y2526	P2429	M2351		S2179	
	T2527		K2352	Q2267		
	Q2528	R2435	Q2353	L2268	S2185	D2090
		N2436	K2354		R2186	P2091
		H2437	F2354		G2187	K2092
K2558		R2438	F2355		N2188	A2093
					W2189	
					G2190	L2097
K2559						
K2560						
K2561						
K2562						
K2563						
K2564						
K2565						
K2566						
K2567						
K2568						
K2569						
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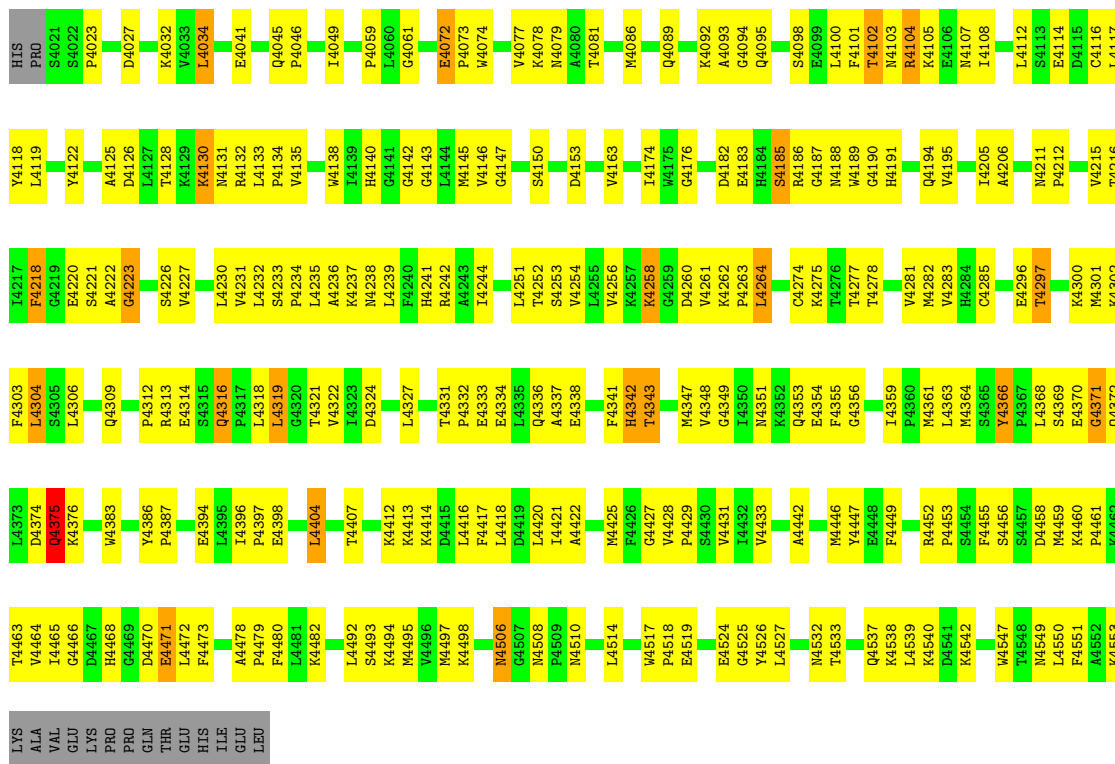
- Molecule 1: liver Carboxylesterase I

Chain I:  49% 44% 5%

[illegible]

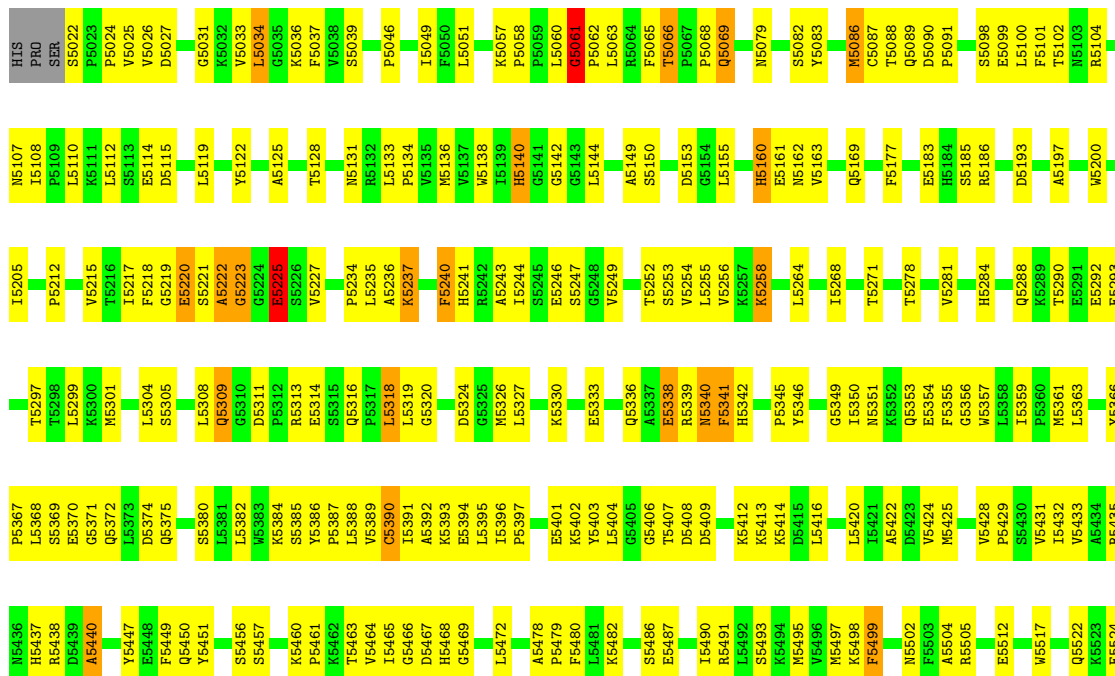
- Molecule 1: liver Carboxylesterase I

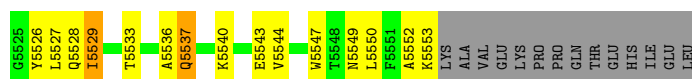
Chain J:



- Molecule 1: liver Carboxylesterase I

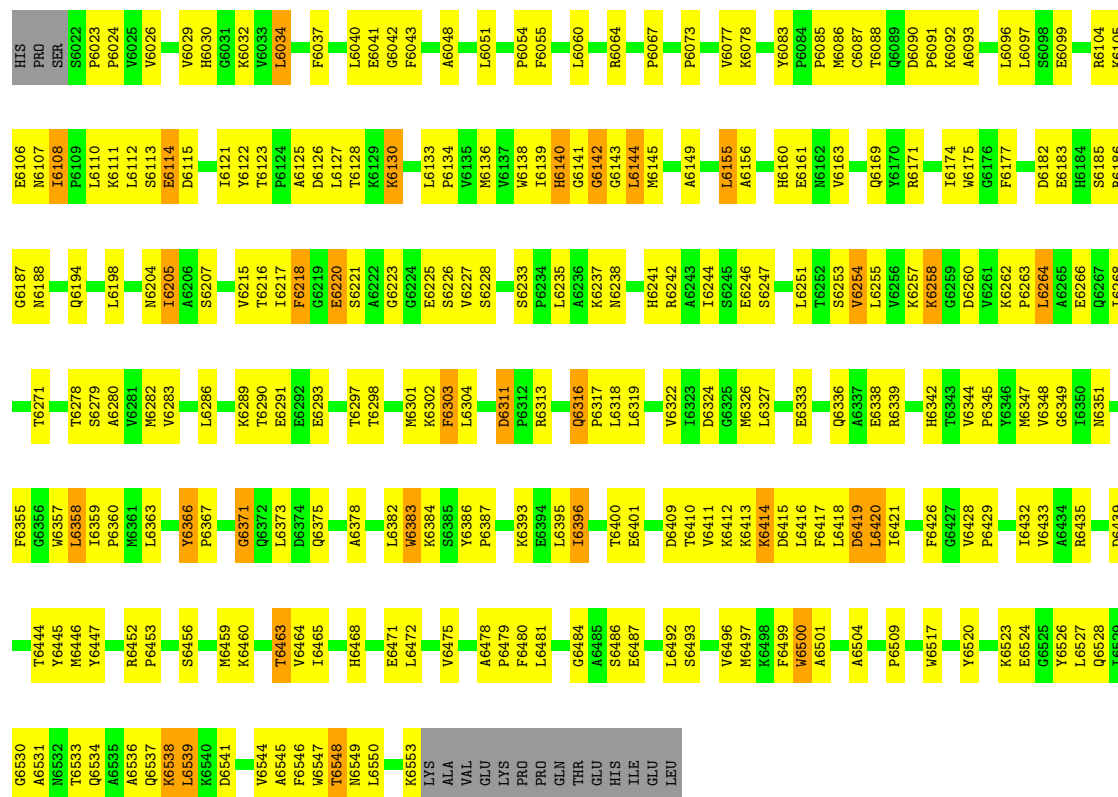
Chain K:





• Molecule 1: liver Carboxylesterase I

Chain L: 51% 41% 5%



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	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 ²)	44.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.46	0/4236	0.98	15/5754 (0.3%)
1	B	0.51	0/4236	1.02	17/5754 (0.3%)
1	C	0.52	1/4230 (0.0%)	0.99	15/5746 (0.3%)
1	D	0.50	0/4241	0.97	10/5761 (0.2%)
1	E	0.49	0/4230	0.98	16/5746 (0.3%)
1	F	0.47	0/4230	1.00	17/5746 (0.3%)
1	G	0.45	0/4236	0.94	11/5754 (0.2%)
1	H	0.48	0/4230	1.03	19/5746 (0.3%)
1	I	0.44	0/4230	0.95	11/5746 (0.2%)
1	J	0.49	0/4236	0.96	7/5754 (0.1%)
1	K	0.44	0/4230	0.96	13/5746 (0.2%)
1	L	0.45	0/4230	0.97	15/5746 (0.3%)
All	All	0.47	1/50795 (0.0%)	0.98	166/68999 (0.2%)

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	3364	MET	SD-CE	7.77	1.99	1.79

All (166) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	6140	HIS	N-CA-C	11.19	124.53	111.11
1	B	2075	SER	N-CA-C	11.15	125.41	111.69
1	B	2339	ARG	N-CA-C	9.53	125.50	111.02
1	E	5075	SER	N-CA-C	8.86	124.50	112.90
1	A	1075	SER	N-CA-C	8.24	121.83	111.69
1	C	3066	THR	CA-C-N	-8.16	113.78	119.66
1	C	3066	THR	C-N-CA	-8.16	113.78	119.66
1	C	3075	SER	N-CA-C	8.05	123.22	113.23
1	J	4114	GLU	N-CA-C	-7.72	103.74	113.01
1	H	2311	ASP	CA-C-N	7.71	126.99	118.97
1	H	2311	ASP	C-N-CA	7.71	126.99	118.97
1	E	5507	GLY	N-CA-C	-7.58	105.28	115.36
1	F	6075	SER	N-CA-C	7.35	120.73	111.69
1	H	2371	GLY	N-CA-C	-7.32	105.88	115.47
1	H	2470	ASP	N-CA-C	7.20	120.04	111.33
1	A	1222	ALA	N-CA-C	-7.16	103.47	111.28
1	K	5537	GLN	N-CA-C	6.90	119.06	108.30
1	E	5233	SER	N-CA-C	6.87	119.58	109.62
1	B	2338	GLU	N-CA-C	-6.81	100.36	110.23
1	K	5061	GLY	CA-C-N	6.70	126.65	119.28
1	K	5061	GLY	C-N-CA	6.70	126.65	119.28
1	H	2316	GLN	CA-C-N	6.67	126.26	119.19
1	H	2316	GLN	C-N-CA	6.67	126.26	119.19
1	I	3339	ARG	N-CA-C	-6.61	104.79	112.86
1	H	2342	HIS	N-CA-C	6.60	118.90	108.67
1	I	3023	PRO	CA-C-N	6.56	126.32	119.76
1	I	3023	PRO	C-N-CA	6.56	126.32	119.76
1	H	2061	GLY	CA-C-N	6.56	126.80	119.32
1	H	2061	GLY	C-N-CA	6.56	126.80	119.32
1	A	1316	GLN	CA-C-N	6.55	126.24	119.56
1	A	1316	GLN	C-N-CA	6.55	126.24	119.56
1	D	4342	HIS	N-CA-C	6.51	119.42	108.23
1	F	6108	ILE	CA-C-N	6.50	126.45	119.76
1	F	6108	ILE	C-N-CA	6.50	126.45	119.76
1	F	6160	HIS	N-CA-C	6.49	118.02	111.07
1	H	2502	ASN	N-CA-C	-6.46	104.32	111.36
1	F	6144	LEU	N-CA-C	-6.44	105.01	112.86
1	L	6114	GLU	N-CA-C	-6.39	105.48	113.28
1	J	4223	GLY	N-CA-C	-6.36	104.79	112.49
1	F	6507	GLY	N-CA-C	-6.36	105.29	115.08
1	B	2318	LEU	N-CA-C	6.33	119.04	109.41
1	G	1233	SER	N-CA-C	6.33	117.63	109.65
1	G	1419	ASP	N-CA-C	-6.30	104.47	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	4356	GLY	N-CA-C	6.26	120.25	112.73
1	K	5160	HIS	N-CA-C	6.25	119.76	111.75
1	C	3316	GLN	CA-C-N	6.24	125.86	119.56
1	C	3316	GLN	C-N-CA	6.24	125.86	119.56
1	E	5114	GLU	N-CA-C	-6.24	104.37	112.23
1	F	6356	GLY	N-CA-C	6.23	120.18	112.64
1	D	4254	VAL	N-CA-C	6.22	118.86	111.09
1	F	6484	GLY	N-CA-C	6.20	123.92	115.00
1	J	4337	ALA	N-CA-C	-6.17	104.47	111.14
1	D	4375	GLN	N-CA-C	6.14	118.76	111.33
1	B	2061	GLY	CA-C-N	6.14	125.76	119.56
1	B	2061	GLY	C-N-CA	6.14	125.76	119.56
1	B	2320	GLY	N-CA-C	6.11	121.33	112.60
1	F	6114	GLU	N-CA-C	-6.10	105.67	113.23
1	F	6291	GLU	N-CA-C	-6.10	103.80	111.11
1	C	3114	GLU	N-CA-C	-6.08	104.77	111.82
1	K	5301	MET	N-CA-C	-6.04	105.40	112.89
1	G	1358	LEU	N-CA-C	6.03	117.54	110.97
1	D	4114	GLU	N-CA-C	-6.00	104.67	112.23
1	C	3531	ALA	N-CA-C	-5.99	104.75	111.28
1	H	2114	GLU	N-CA-C	-5.97	105.25	112.54
1	K	5440	ALA	N-CA-C	-5.96	106.06	113.15
1	D	4419	ASP	N-CA-C	-5.95	104.80	111.28
1	E	5396	ILE	CB-CA-C	-5.95	108.05	113.70
1	K	5529	ILE	N-CA-C	5.94	117.29	109.21
1	A	1205	ILE	N-CA-C	5.92	117.37	110.62
1	G	1114	GLU	N-CA-C	-5.89	105.59	112.89
1	C	3160	HIS	N-CA-C	5.86	117.75	111.36
1	G	1224	GLY	N-CA-C	-5.81	105.46	112.49
1	A	1396	ILE	CB-CA-C	-5.81	108.18	113.70
1	J	4458	ASP	N-CA-C	-5.79	106.05	113.23
1	L	6366	TYR	CA-C-N	5.79	127.07	119.84
1	L	6366	TYR	C-N-CA	5.79	127.07	119.84
1	E	5366	TYR	CA-C-N	5.78	127.07	119.84
1	E	5366	TYR	C-N-CA	5.78	127.07	119.84
1	L	6371	GLY	N-CA-C	-5.78	105.69	115.34
1	B	2108	ILE	N-CA-C	5.77	112.81	107.56
1	I	3253	SER	N-CA-C	5.75	119.77	112.87
1	G	1311	ASP	CA-C-N	5.73	125.59	119.28
1	G	1311	ASP	C-N-CA	5.73	125.59	119.28
1	C	3199	ARG	N-CA-C	-5.69	105.06	112.23
1	K	5222	ALA	N-CA-C	-5.69	105.08	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1086	MET	N-CA-C	-5.67	101.04	110.17
1	A	1254	VAL	N-CA-C	5.66	120.36	112.50
1	F	6316	GLN	CA-C-N	5.64	125.48	119.28
1	F	6316	GLN	C-N-CA	5.64	125.48	119.28
1	K	5031	GLY	N-CA-C	5.63	118.60	111.85
1	K	5225	GLU	N-CA-C	-5.62	104.79	111.03
1	L	6548	THR	N-CA-C	-5.62	104.56	111.75
1	F	6254	VAL	N-CA-C	5.61	117.01	110.62
1	H	2425	MET	N-CA-C	5.58	117.05	111.07
1	E	5227	VAL	N-CA-C	-5.58	104.93	110.62
1	B	2183	GLU	N-CA-C	5.55	119.55	112.34
1	B	2221	SER	CB-CA-C	-5.52	109.73	117.23
1	I	3366	TYR	CA-C-N	5.51	126.73	119.84
1	I	3366	TYR	C-N-CA	5.51	126.73	119.84
1	E	5291	GLU	N-CA-C	-5.51	105.17	111.07
1	I	3140	HIS	N-CA-C	5.51	117.64	110.43
1	A	1507	GLY	N-CA-C	-5.49	107.68	115.30
1	A	1193	ASP	N-CA-C	-5.45	105.34	111.28
1	E	5083	TYR	N-CA-C	5.45	116.27	109.57
1	H	2072	GLU	CA-C-N	5.43	125.36	119.76
1	H	2072	GLU	C-N-CA	5.43	125.36	119.76
1	K	5140	HIS	N-CA-C	5.42	117.08	110.41
1	L	6144	LEU	N-CA-C	-5.42	105.30	112.24
1	E	5537	GLN	N-CA-C	5.42	117.42	109.24
1	B	2233	SER	N-CA-C	5.40	116.46	109.65
1	A	1233	SER	N-CA-C	5.40	116.88	110.07
1	D	4224	GLY	N-CA-C	-5.40	106.24	112.50
1	D	4160	HIS	N-CA-C	5.39	117.24	111.36
1	D	4510	ASN	N-CA-C	5.39	117.69	110.35
1	C	3440	ALA	N-CA-C	-5.39	106.48	113.16
1	K	5223	GLY	N-CA-C	-5.35	105.92	112.77
1	B	2491	ARG	N-CA-C	-5.33	105.16	110.97
1	B	2428	VAL	CB-CA-C	-5.33	108.71	114.35
1	A	1311	ASP	CA-C-N	5.30	125.62	119.47
1	A	1311	ASP	C-N-CA	5.30	125.62	119.47
1	A	1023	PRO	N-CA-C	5.28	117.14	110.70
1	C	3223	GLY	N-CA-C	-5.28	105.95	113.86
1	C	3337	ALA	N-CA-C	-5.26	105.66	111.71
1	F	6049	ILE	N-CA-C	5.26	115.67	107.99
1	G	1221	SER	CB-CA-C	-5.23	109.02	116.34
1	H	2165	VAL	N-CA-C	5.22	115.83	108.36
1	E	5484	GLY	N-CA-C	5.22	123.15	113.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1180	THR	N-CA-C	-5.22	106.31	113.30
1	J	4506	ASN	N-CA-C	5.21	119.39	112.30
1	B	2343	THR	N-CA-C	5.21	117.85	110.50
1	F	6452	ARG	CA-C-N	5.21	125.14	119.78
1	F	6452	ARG	C-N-CA	5.21	125.14	119.78
1	H	2297	THR	N-CA-C	-5.21	105.69	111.36
1	I	3297	THR	N-CA-C	-5.19	105.30	111.69
1	B	2502	ASN	N-CA-C	-5.18	105.81	111.82
1	H	2253	SER	N-CA-C	5.17	121.82	110.80
1	G	1452	ARG	CA-C-N	5.17	125.11	119.78
1	G	1452	ARG	C-N-CA	5.17	125.11	119.78
1	I	3510	ASN	N-CA-C	5.17	117.79	110.50
1	J	4186	ARG	N-CA-C	5.16	117.57	111.33
1	B	2324	ASP	N-CA-C	5.15	117.64	111.71
1	C	3508	ASN	CA-C-N	5.14	124.93	119.28
1	C	3508	ASN	C-N-CA	5.14	124.93	119.28
1	L	6396	ILE	CB-CA-C	-5.13	108.91	114.35
1	E	5023	PRO	CA-C-N	5.13	125.53	119.99
1	E	5023	PRO	C-N-CA	5.13	125.53	119.99
1	D	4537	GLN	N-CA-C	5.13	117.04	108.99
1	L	6383	TRP	N-CA-C	-5.13	105.34	111.03
1	H	2222	ALA	N-CA-C	-5.12	105.82	111.71
1	L	6311	ASP	CA-C-N	5.12	124.91	119.28
1	L	6311	ASP	C-N-CA	5.12	124.91	119.28
1	D	4358	LEU	N-CA-C	5.09	117.23	111.02
1	L	6316	GLN	CA-C-N	5.09	124.88	119.28
1	L	6316	GLN	C-N-CA	5.09	124.88	119.28
1	L	6228	SER	N-CA-C	-5.09	105.42	110.97
1	E	5221	SER	CB-CA-C	-5.09	110.72	116.63
1	H	2454	SER	N-CA-C	-5.07	107.12	113.15
1	C	3221	SER	CB-CA-C	-5.06	110.34	117.23
1	G	1437	HIS	N-CA-C	-5.06	105.76	111.28
1	B	2086	MET	N-CA-C	-5.05	102.30	110.32
1	F	6076	PHE	N-CA-C	5.04	113.59	108.75
1	I	3324	ASP	N-CA-C	5.04	117.67	111.82
1	E	5069	GLN	N-CA-C	5.04	117.81	110.10
1	K	5318	LEU	N-CA-C	5.03	115.68	108.74
1	L	6108	ILE	N-CA-C	5.02	113.39	107.77
1	I	3343	THR	N-CA-C	5.00	117.72	110.42

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	244	0
1	B	4130	0	4132	195	0
1	C	4124	0	4127	186	0
1	D	4135	0	4134	174	0
1	E	4124	0	4127	212	0
1	F	4124	0	4127	208	0
1	G	4130	0	4132	254	0
1	H	4124	0	4127	204	0
1	I	4124	0	4127	241	0
1	J	4130	0	4134	226	0
1	K	4124	0	4127	239	0
1	L	4124	0	4127	260	0
2	A	28	0	26	3	0
2	B	14	0	13	5	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
3	A	25	0	23	21	0
3	B	25	0	23	21	0
3	C	25	0	19	28	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	31	0
3	I	25	0	24	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	9	0
4	G	69	0	0	9	0
4	H	95	0	0	10	0
4	I	80	0	0	10	0
4	J	110	0	0	9	0
4	K	73	0	0	11	0
4	L	75	0	0	16	0
All	All	51134	0	49998	2599	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 26.

All (2599) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3242:ARG:HG2	1:C:3242:ARG:HH11	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:B:2359:ILE:HG12	3:B:2:N LX:H71	1.51	0.92
1:I:3490:ILE:HG22	1:I:3494:LYS:HD2	1.49	0.92
1:K:5237:LYS:HA	1:K:5237:LYS:HE2	1.49	0.92
1:E:5363:LEU:CB	3:E:5:N LX:H201	1.99	0.92
1:H:2359:ILE:HG23	3:H:2:N LX:H82	1.49	0.92
1:J:4363:LEU:HD13	3:J:4:N LX:H181	1.52	0.92
1:E:5304:LEU:HD13	3:E:5:N LX:H181	1.52	0.92
1:B:2091:PRO:HG3	1:B:2112:LEU:HD11	1.51	0.91
1:D:4215:VAL:H	1:D:4241:HIS:HD2	1.14	0.91
1:G:1079:ASN:HB2	2:G:179:NAG:H82	1.50	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:N LX: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:N LX:H201	1.51	0.89
1:H:2404:LEU:HB3	1:H:2413:LYS:HG3	1.53	0.89
1:A:1134:PRO:HG2	1:A:1163:VAL:HG12	1.53	0.89
1:C:3143:GLY:HA3	3:C:3:N LX:H152	1.52	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:N LX: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:G:1396:ILE:HB	1:G:1397:PRO:HD3	1.56	0.86
1:H:2304:LEU:CB	3:H:2:N LX:H201	2.05	0.86
1:E:5091:PRO:HG3	1:E:5112:LEU:HD11	1.57	0.86
1:D:4421:ILE:HG22	1:D:4425:MET:HE2	1.56	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:S ER:OG	3:K:5:N LX:H71	1.78	0.84
1:E:5490:I LE:O	1:E:5494:L YS:HG3	1.76	0.84
1:K:5221:S ER:OG	1:K:5222:A LA:N	2.09	0.84
1:D:4292:G LU:O	1:D:4296:G LU: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:V AL:H	1:L:6241:H IS:CD2	1.96	0.83
1:C:3257:L YS:HD3	4:C:7152:H OH:O	1.78	0.82
1:J:4468:H IS:NE2	3:J:4:N LX:H21	1.94	0.82
1:A:1353:G LN:NE2	1:A:1465:I LE:H	1.77	0.82
1:A:1414:L YS:NZ	1:F:6370:G LU:HA	1.93	0.82
1:F:6034:LEU:HD12	1:F:6079:A SN:ND2	1.93	0.82
1:H:2263:P RO:O	1:H:2267:G LN:HG3	1.79	0.82
1:I:3370:G LU:HG3	1:J:4461:P RO:HG3	1.59	0.82
1:L:6086:M ET:HE2	1:L:6110:LEU:HB2	1.60	0.82
1:A:1461:P RO:HG2	1:A:1464:V AL:HG23	1.62	0.82
1:L:6023:P RO:HB2	1:L:6034:LEU:HD21	1.61	0.82
1:D:4242:A RG:HG2	1:D:4242:A RG: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:C:3268:I LE:HG12	1:C:3301:M ET:HE2	1.63	0.81
1:E:5086:M ET:HE3	1:E:5089:G LN:CD	2.06	0.81
1:H:2363:LEU:HD13	3:H:2:N LX:H101	1.62	0.81
1:A:1086:M ET:HE3	1:A:1110:LEU:HB2	1.61	0.81
1:A:1331:T HR:OG1	1:A:1334:G LU:HG2	1.79	0.81
1:H:2221:S ER:HB3	3:H:2:N LX:O1	1.81	0.81
1:L:6105:L YS:HD3	1:L:6106:G LU:HG3	1.60	0.81
1:C:3088:T HR: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:A SP:OD2	1:L:6280:A LA:HB3	1.81	0.81
1:C:3364:M ET:HE3	3:C:3:N LX:H181	1.60	0.81
1:F:6254:V AL:HG21	3:F:6:N LX:O1	1.80	0.81
1:J:4421:I LE:HG22	1:J:4425:M ET:HE2	1.61	0.81
1:C:3343:T HR:HB	1:C:3442:A LA:HB2	1.62	0.80
1:I:3512:G LU:CD	1:I:3512:G LU:H	1.86	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
1:C:3364:M ET:SD	3:C:3:N LX:H181	2.22	0.80
1:A:1304:LEU:HB3	3:A:1:N LX:H203	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1092:LYS:HE3	4:A:8088:HOH:O	1.83	0.79
1:A:1375:GLN:HE22	1:A:1400:THR:HG22	1.47	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:A:1376:LYS:HD3	1:F:6462:LYS:HE2	1.62	0.78
1:I:3462:LYS:HZ1	1:J:4376:LYS:HZ2	1.28	0.78
1:L:6258:LYS:H	1:L:6258:LYS:HD3	1.45	0.78
1:B:2079:ASN:HD22	2:B:279:NAG:H82	1.49	0.78
1:I:3318:LEU:HG	3:I:3:NLX:C19	2.12	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:A:1363:LEU:HD22	3:A:1:NLX:H181	1.64	0.77
1:L:6304:LEU:HD22	3:L:6:NLX:H172	1.64	0.77
1:I:3234:PRO:O	1:I:3237:LYS:HG2	1.85	0.77
1:J:4132:ARG:HH12	1:J:4206:ALA:CB	1.98	0.77
1:J:4215:VAL:H	1:J:4241:HIS:HD2	1.33	0.77
1:L:6114:GLU:OE1	1:L:6291:GLU:HB2	1.84	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:1086:MET:HE3	1:G:1148:ALA:HB2	1.68	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:D:4471:GLU:O	1:D:4475:VAL:HG23	1.85	0.76
1:D:4538:LYS:HD3	1:D:4541:ASP:OD1	1.86	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:D:4349:GLY:HA3	1:D:4447:TYR:CZ	2.20	0.75
1:I:3428:VAL:HB	1:I:3429:PRO:HD3	1.68	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:F:6452:ARG:HB2	1:F:6465:ILE:HG12	1.69	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:J:4059:PRO:HD3	1:J:4117:LEU:HD12	1.69	0.74
3:C:3:N LX:C9	3:C:3:N LX:C17	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:D:4421:ILE:CG2	1:D:4425:MET:HE2	2.16	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:F:6257:LYS:HA	1:F:6257:LYS:HE3	1.70	0.74
1:H:2371:GLY:HA2	1:H:2414:LYS:HD3	1.68	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: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:J:4251:LEU:HD11	1:J:4336:GLN:HE22	1.52	0.73
1:J:4304:LEU:HG	3:J:4:N LX:H203	1.70	0.73
1:B:2359:ILE:HB	1:B:2360:PRO:CD	2.19	0.73
1:I:3142:GLY:HA2	3:I:3:N LX:H71	1.70	0.73
1:K:5363:LEU:HB2	3:K:5:N LX:H201	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4257:LYS:HZ1	1:D:4316:GLN:HG3	1.52	0.73
1:D:4359:ILE:HB	1:D:4360:PRO:HD3	1.71	0.73
1:D:4304:LEU:HB3	3:D:4:N LX:H201	1.69	0.73
1:G:1215:VAL:H	1:G:1241:HIS:CD2	2.02	0.73
1:F:6235:LEU:HD12	1:F:6327:LEU:HD12	1.70	0.72
1:H:2420:LEU:O	1:H:2424:VAL:HG23	1.89	0.72
1:L:6358:LEU:HG	1:L:6363:LEU:HD12	1.71	0.72
1:B:2304:LEU:HA	3:B:2:N LX:H191	1.71	0.72
1:B:2371:GLY:HA2	1:B:2414:LYS:HD3	1.71	0.72
1:C:3143:GLY:HA3	3:C:3:N LX:C15	2.18	0.72
1:E:5235:LEU:HD12	1:E:5327:LEU:HA	1.70	0.72
1:F:6097:LEU:CD2	3:F:6:N LX:H192	2.18	0.72
1:K:5396:ILE:HB	1:K:5397:PRO:HD3	1.69	0.72
1:J:4260:ASP:OD2	1:J:4263:PRO:HD3	1.89	0.72
1:D:4363:LEU:HB3	3:D:4:N LX:C18	2.18	0.72
1:B:2083:TYR:CE2	1:B:2108:ILE:HD13	2.25	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:F:6359:ILE:HB	1:F:6360:PRO:HD3	1.71	0.72
1:A:1095:GLN:O	1:A:1099:GLU:HG3	1.90	0.72
1:E:5308:LEU:HD21	1:E:5367:PRO:HG3	1.70	0.72
1:C:3249:VAL:HG23	1:C:3251:LEU:H	1.55	0.72
1:D:4354:GLU:O	1:D:4468:HIS:HB2	1.90	0.72
1:E:5308:LEU:HD21	1:E:5367:PRO:CG	2.20	0.71
1:K:5086:MET:HE3	1:K:5089:GLN:CD	2.14	0.71
1:A:1237:LYS:HG2	1:A:1238:ASN:ND2	2.05	0.71
1:L:6550:LEU:HA	1:L:6553:LYS:HZ3	1.54	0.71
3:C:3:N LX:C9	3:C:3:N LX: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:A:1104:ARG:CZ	1:A:1153:ASP:HB2	2.20	0.71
1:F:6034:LEU:HD12	1:F:6079:ASN:HD22	1.53	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: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:K:5359:ILE:HG23	3:K:5:N LX:H152	1.71	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:2121:ILE:HD13	1:H:2166:VAL:HG22	1.73	0.70
1:E:5304:LEU:HB3	3:E:5:N LX:C18	2.21	0.70
1:K:5024:PRO:HD3	1:K:5037:PHE:CD1	2.27	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:H:2158:ALA:HB2	1:H:2165:VAL:HG23	1.72	0.70
4:B:7643:HOH:O	1:E:5092:LYS:HD2	1.91	0.70
1:C:3319:LEU:HA	4:C:7152:HOH:O	1.92	0.70
1:E:5363:LEU:HB2	3:E:5:N LX:H201	1.74	0.70
1:H:2359:ILE:HD13	3:H:2:N LX:H71	1.72	0.70
1:I:3268:ILE:HG12	1:I:3301:MET:HE2	1.74	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:F:6268:ILE:HG12	1:F:6301:MET:HE2	1.73	0.69
1:A:1215:VAL:H	1:A:1241:HIS:CD2	2.04	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: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:A:1349:GLY:HA3	1:A:1447:TYR:CE1	2.27	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:K:5082:SER:HB2	4:K:7929:HOH:O	1.92	0.69
1:L:6373:LEU:HB2	1:L:6414:LYS:HB3	1.75	0.69
1:D:4343:THR:HA	4:D:7962:HOH:O	1.92	0.69
1:G:1404:LEU:HB3	1:G:1413:LYS:HG3	1.74	0.69
1:G:1425:MET:HE3	1:G:1426:PHE:HE1	1.58	0.69
1:I:3491:ARG:HA	1:I:3494:LYS:HD3	1.74	0.69
1:G:1385:SER:O	1:G:1389:VAL:HG22	1.93	0.69
1:H:2258:LYS:HD2	4:H:7424:HOH:O	1.92	0.69
1:I:3242:ARG:HG2	1:I:3242:ARG:HH11	1.58	0.69
1:L:6262:LYS:O	1:L:6266:GLU:HG2	1.93	0.69
1:B:2227:VAL:O	1:B:2231:VAL:HG23	1.91	0.69
1:E:5464:VAL:C	1:E:5465:ILE:HD12	2.17	0.69
1:L:6260:ASP:HA	4:L:7557:HOH:O	1.93	0.69
1:L:6359:ILE:HB	1:L:6360:PRO:HD3	1.73	0.69
1:C:3132:ARG:HB3	1:C:3211:ASN:HB2	1.74	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:F:6395:LEU:HB3	1:F:6550:LEU:HD21	1.73	0.69
1:G:1429:PRO:O	1:G:1433:VAL:HG23	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:5420:LEU:HD12	1:K:5547:TRP:HZ2	1.58	0.69
1:L:6215:VAL:N	1:L:6241:HIS:HD2	1.91	0.69
1:L:6257:LYS:HE2	1:L:6316:GLN:NE2	2.08	0.69
1:L:6355:PHE:CE1	1:L:6360:PRO:HG3	2.27	0.69
1:A:1527:LEU:HD11	1:A:1533:THR:HG22	1.74	0.69
1:C:3057:LYS:HD3	1:C:3063:LEU:HD11	1.75	0.69
1:G:1304:LEU:CD1	1:G:1318:LEU:HD23	2.23	0.69
1:I:3217:ILE:HG13	1:I:3217:ILE:O	1.92	0.69
1:C:3370:GLU:HG3	1:D:4461:PRO:HG3	1.73	0.68
3:C:3:NLX:C14	3:C:3:NLX:C10	2.71	0.68
1:C:3428:VAL:HB	1:C:3429:PRO:HD3	1.74	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:3236:ALA:HA	1:C:3239:LEU:HD12	1.76	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:K:5456:SER:HB3	1:K:5460:LYS:HD3	1.75	0.68
1:C:3290:THR:OG1	1:C:3293:GLU:HG3	1.94	0.68
1:J:4334:GLU:O	1:J:4338:GLU:HG2	1.92	0.68
1:G:1391:ILE:HA	4:G:8113:HOH:O	1.92	0.68
1:H:2221:SER:CB	3:H:2:NLX:O1	2.42	0.68
1:K:5351:ASN:HB3	1:K:5466:GLY:O	1.94	0.68
1:D:4260:ASP:OD1	1:D:4263:PRO:HD3	1.94	0.68
1:F:6024:PRO:HG3	1:F:6037:PHE:CE1	2.28	0.68
1:H:2363:LEU:HD13	3:H:2:NLX:C10	2.23	0.68
1:I:3088:THR:HG22	1:I:3295:LEU:HD13	1.76	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:J:4525:GLY:HA2	1:J:4537:GLN:HG2	1.76	0.67
1:L:6271:THR:HG22	1:L:6297:THR:HG23	1.76	0.67
1:L:6545:ALA:O	1:L:6548:THR:HG22	1.95	0.67
1:A:1372:GLN:HB2	1:A:1410:THR:HG22	1.75	0.67
1:A:1385:SER:O	1:A:1389:VAL:HG22	1.95	0.67
1:B:2174:ILE:HG13	4:B:7012:HOH:O	1.95	0.67
1:F:6174:ILE:HG13	4:F:7076:HOH:O	1.95	0.67
1:F:6220:GLU:HG2	1:F:6472:LEU:HD21	1.77	0.67
1:F:6353:GLN:HE22	1:F:6465:ILE:H	1.40	0.67
1:H:2386:TYR:N	1:H:2387:PRO:HD2	2.09	0.67
1:L:6254:VAL:HG22	1:L:6318:LEU:HD12	1.75	0.67
1:A:1376:LYS:HD3	1:F:6462:LYS:CE	2.24	0.67
1:F:6043:PHE:HA	4:F:7849:HOH:O	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:5498:LYS:HG2	1:K:5502:ASN:HD21	1.60	0.67
1:L:6087:CYS:HB3	4:L:7703:HOH:O	1.95	0.67
1:A:1363:LEU:CD2	3:A:1:N LX:H181	2.25	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:K:5290:THR:OG1	1:K:5293:GLU:HG3	1.95	0.67
1:F:6097:LEU:HB2	3:F:6:N LX:H192	1.77	0.67
1:I:3317:PRO:HG2	3:I:3:N LX:C19	2.25	0.67
1:I:3324:ASP:OD1	1:I:3326:MET:HB2	1.94	0.67
1:J:4215:VAL:H	1:J:4241:HIS:CD2	2.11	0.67
1:H:2186:ARG:HB3	1:H:2324:ASP:HB2	1.77	0.67
1:K:5464:VAL:C	1:K:5465:ILE:HD12	2.20	0.67
1:C:3227:VAL:O	1:C:3231:VAL:HG23	1.94	0.67
1:E:5125:ALA:HB1	1:E:5131:ASN:ND2	2.10	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:N LX:C10	2.24	0.66
1:B:2304:LEU:HA	3:B:2:N LX: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:N LX: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:G:1142:GLY:HA2	3:G:1:N LX:H152	1.76	0.66
1:G:1146:VAL:HG21	3:G:1:N LX:H162	1.77	0.66
1:K:5221:SER:HB2	3:K:5:N LX:O3	1.95	0.66
1:L:6141:GLY:N	4:L:7115:HOH:O	2.22	0.66
1:L:6447:TYR:C	1:L:6447:TYR:CD2	2.74	0.66
1:A:1086:MET:HE2	1:A:1110:LEU:HD12	1.77	0.66
1:E:5145:MET:HB2	1:E:5304: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:H:2498:LYS:HG2	1:H:2514:LEU:HD11	1.76	0.66
1:J:4132:ARG:HH12	1:J:4206:ALA:HB1	1.59	0.66
1:L:6216:THR:HG23	1:L:6242:ARG:HB2	1.78	0.66
1:L:6257:LYS:HE2	1:L:6316:GLN:CD	2.21	0.66
1:C:3498:LYS:HB3	1:C:3514:LEU:HD11	1.75	0.66
1:E:5409:ASP:OD2	1:E:5411:VAL:HB	1.96	0.66
1:F:6143:GLY:N	3:F:6:N LX:H82	2.11	0.66
1:F:6258:LYS:HE2	1:F:6258:LYS:O	1.95	0.66
1:I:3412:LYS:O	1:I:3416:LEU:HG	1.95	0.66
1:J:4221:SER:OG	1:J:4222:ALA:N	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:4396:ILE:HB	1:J:4397:PRO:HD3	1.77	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:L:6395:LEU:HD22	1:L:6550:LEU:HD11	1.77	0.66
1:J:4191:HIS:O	1:J:4195:VAL:HG23	1.95	0.66
1:A:1232:LEU:HD23	1:A:1341:PHE:HB3	1.78	0.66
1:C:3407:THR:HG21	1:C:3412:LYS:NZ	2.11	0.66
1:D:4303:PHE:O	1:D:4304:LEU:HB2	1.95	0.66
1:E:5279:SER:HA	1:E:5282:MET:HE3	1.76	0.66
1:E:5304:LEU:HD21	1:E:5318:LEU:CD2	2.26	0.66
1:G:1146:VAL:CG2	3:G:1:NLX:H162	2.26	0.66
1:J:4364:MET:SD	3:J:4:NLX:H72	2.35	0.66
1:K:5104:ARG:NH1	1:K:5153:ASP:HB2	2.10	0.66
1:L:6024:PRO:HA	4:L:7722:HOH:O	1.96	0.66
1:A:1428:VAL:HB	1:A:1429:PRO:HD3	1.78	0.65
1:E:5134:PRO:HG2	1:E:5163:VAL:HG12	1.78	0.65
1:G:1220:GLU:HA	1:G:1246:GLU:O	1.97	0.65
1:K:5218:PHE:HB2	1:K:5244:ILE:HB	1.77	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
3:F:6:NLX:O4	4:F:7502:HOH:O	2.13	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:E:5395:LEU:HB3	1:E:5550:LEU:HD11	1.78	0.65
1:G:1363:LEU:HD13	3:G:1:NLX:H102	1.78	0.65
1:J:4304:LEU:HG	3:J:4:NLX:C20	2.26	0.65
1:D:4395:LEU:HD13	1:D:4550:LEU:HG	1.78	0.65
1:I:3125:ALA:HB2	1:I:3133:LEU:HD11	1.79	0.65
1:I:3447:TYR:HB3	1:I:3517:TRP:CZ2	2.31	0.65
1:G:1276:THR:HG22	1:G:1282:MET:SD	2.36	0.65
1:H:2370:GLU:C	1:H:2372:GLN:H	2.03	0.65
1:J:4549:ASN:HB2	4:J:8096:HOH:O	1.95	0.65
1:E:5149:ALA:HB1	1:E:5167:THR:HB	1.79	0.65
1:J:4104:ARG:NH1	1:J:4153:ASP:HB2	2.12	0.65
1:L:6139:ILE:HG22	4:L:7115:HOH:O	1.96	0.65
1:B:2359:ILE:HG23	3:B:2:NLX:C8	2.25	0.65
1:C:3357:TRP:O	1:C:3360:PRO:HD2	1.96	0.65
1:D:4330:LYS:HG3	1:D:4335:LEU:HG	1.78	0.65
1:E:5290:THR:OG1	1:E:5293:GLU:HG3	1.95	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:6024:PRO:HG3	1:L:6037:PHE:CE1	2.31	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: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
1:J:4461:PRO:HG2	1:J:4464:VAL:HG23	1.79	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:6252:THR:HG23	1:F:6425:MET:O	1.96	0.64
1:C:3364:MET:HE3	3:C:3:NLX:C18	2.28	0.64
1:F:6456:SER:HB3	1:F:6460:LYS:HD3	1.78	0.64
1:K:5495:MET:HE1	1:K:5533:THR:OG1	1.98	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: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:F:6221:SER:OG	3:F:6:NLX:H72	1.98	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:A:1372:GLN:C	1:A:1373:LEU:HD12	2.23	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:I:3486:SER:O	1:I:3490:ILE:HG13	1.98	0.64
1:D:4251:LEU:HD21	1:D:4333:GLU:HG3	1.80	0.63
1:G:1435:ARG:NH1	1:G:1544:VAL:HG11	2.12	0.63
1:J:4098:SER:O	1:J:4102:THR:HG22	1.97	0.63
1:J:4130:LYS:HE2	1:J:4132:ARG:NE	2.13	0.63
1:K:5311:ASP:HB3	1:K:5314:GLU:HG2	1.80	0.63
1:L:6414:LYS:HE2	1:L:6415:ASP:OD2	1.97	0.63
1:I:3452:ARG:HB2	1:I:3465:ILE:HG12	1.79	0.63
1:J:4421:ILE:CG2	1:J:4425:MET:HE2	2.28	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: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:E:5340:ASN:ND2	1:E:5342:HIS:H	1.96	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:1264:LEU:HG	1:A:1316:GLN:HG2	1.80	0.63
1:F:6258:LYS:HE2	1:F:6258:LYS:H	1.64	0.63
1:L:6051:LEU:HD13	1:L:6083:TYR:CE1	2.33	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:E:5523:LYS:O	1:E:5538:LYS:HE3	1.98	0.63
1:F:6478:ALA:HB3	1:F:6479:PRO:HD3	1.79	0.63
1:I:3142:GLY:CA	3:I:3:NLX:H71	2.29	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
1:A:1304:LEU:CD1	1:A:1318:LEU:HD23	2.29	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:G:1279:SER:O	1:G:1283:VAL:HG23	1.98	0.63
1:D:4126:ASP:H	1:D:4131:ASN:ND2	1.96	0.63
1:F:6138:TRP:CZ3	1:F:6219:GLY:HA2	2.34	0.63
1:H:2235:LEU:HD12	1:H:2327:LEU:HA	1.80	0.63
1:H:2526:TYR:CE1	1:H:2539:LEU:HD13	2.34	0.63
1:J:4079:ASN:HD21	2:J:479:NAG:H5	1.63	0.63
1:D:4461:PRO:HG2	1:D:4464:VAL:HG23	1.80	0.63
1:G:1092:LYS:NZ	1:L:6302:LYS:HB2	2.13	0.63
1:G:1409:ASP:HB3	1:G:1412:LYS:HB2	1.80	0.63
1:J:4407:THR:HG21	1:J:4412:LYS:HD2	1.81	0.63
1:K:5324:ASP:OD1	1:K:5326:MET:HB2	1.99	0.63
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:C:3431:VAL:HA	1:C:3446:MET:HE1	1.80	0.62
3:C:3:NLX:C9	3:C:3:NLX:C13	2.76	0.62
1:D:4423:ASP:OD1	1:D:4540:LYS:HE2	1.99	0.62
1:I:3462:LYS:NZ	1:J:4376:LYS:HZ2	1.97	0.62
1:K:5467:ASP:OD1	1:K:5468:HIS:N	2.30	0.62
1:L:6523:LYS:HB3	1:L:6537:GLN:OE1	1.98	0.62
1:C:3351:ASN:ND2	1:C:3449:PHE:HB3	2.14	0.62
1:E:5188:ASN:O	1:E:5192:LEU:HG	1.99	0.62
1:I:3220:GLU:HG2	4:I:7760:HOH:O	1.99	0.62
1:J:4142:GLY:C	3:J:4:NLX:H152	2.24	0.62
1:J:4354:GLU:O	1:J:4468:HIS:HB2	1.99	0.62
1:E:5089:GLN:OE1	1:E:5146:VAL:HB	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4145:MET:HG3	1:D:4304:LEU:HD11	1.80	0.62
1:A:1359:ILE:HG23	3:A:1:NLX:H71	1.82	0.62
1:C:3324:ASP:OD1	1:C:3326:MET:HB2	1.98	0.62
1:E:5311:ASP:O	1:E:5314:GLU:HG2	1.99	0.62
1:F:6097:LEU:HD13	3:F:6:NLX:H191	1.82	0.62
1:H:2463:THR:HG23	4:H:7113:HOH:O	1.98	0.62
1:B:2241:HIS:C	1:B:2242:ARG:HD2	2.24	0.62
3:C:3:NLX:C20	3:C:3:NLX:H102	2.30	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:J:4333:GLU:H	1:J:4333:GLU:CD	2.07	0.62
1:I:3358:LEU:O	1:I:3363:LEU:HD12	1.99	0.62
1:A:1030:HIS:HB3	1:A:1073:PRO:HA	1.81	0.62
1:F:6304:LEU:HD22	3:F:6:NLX:H101	1.81	0.62
1:G:1471:GLU:O	1:G:1475:VAL:HG23	1.99	0.62
1:H:2304:LEU:HD13	3:H:2:NLX:H171	1.80	0.62
1:K:5403:TYR:O	1:K:5416:LEU:HD13	1.99	0.62
1:F:6097:LEU:HD11	1:F:6101:PHE:CE2	2.35	0.62
1:K:5220:GLU:O	1:K:5221:SER:HB3	1.99	0.62
1:L:6363:LEU:HB3	3:L:6:NLX:H201	1.79	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:A:1279:SER:O	1:A:1283:VAL:HG23	2.00	0.61
1:H:2426:PHE:C	1:H:2429:PRO:HD2	2.24	0.61
1:J:4251:LEU:HD11	1:J:4336:GLN:NE2	2.14	0.61
1:K:5428:VAL:HB	1:K:5429:PRO:HD3	1.81	0.61
1:A:1308:LEU:HD11	1:A:1367:PRO:HG3	1.82	0.61
1:A:1409:ASP:HB3	1:A:1412:LYS:HB2	1.82	0.61
1:D:4349:GLY:HA3	1:D:4447:TYR:CE1	2.35	0.61
1:G:1395:LEU:HB3	1:G:1550:LEU:HD11	1.83	0.61
1:I:3302:LYS:HD2	1:J:4092:LYS:HD2	1.80	0.61
1:B:2024:PRO:HG3	1:B:2037:PHE:CE1	2.35	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:A:1423:ASP:O	1:A:1428:VAL:HG23	2.01	0.61
1:F:6140:HIS:HD2	1:F:6141:GLY:O	1.83	0.61
1:H:2264:LEU:HD22	1:H:2316:GLN:HE21	1.63	0.61
1:J:4032:LYS:HB2	1:J:4077:VAL:HA	1.82	0.61
1:J:4386:TYR:N	1:J:4387:PRO:HD2	2.16	0.61
1:A:1114:GLU:HG3	1:A:1291:GLU:OE2	2.00	0.61
1:B:2174:ILE:CD1	1:B:2298:THR:HG22	2.29	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:4:NLX:H2O3	3:D:4:NLX:O4	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:I:3258:LYS:HE2	1:I:3258:LYS:H	1.65	0.61
1:J:4231:VAL:O	1:J:4341:PHE:HB2	1.99	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: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
1:I:3144:LEU:HD12	1:I:3320:GLY:HA2	1.82	0.61
1:J:4074:TRP:CE2	1:J:4078:LYS:HE2	2.36	0.61
1:J:4081:THR:OG1	2:J:479:NAG:H5	2.00	0.61
1:L:6363:LEU:HB3	3:L:6:NLX:H162	1.82	0.61
1:B:2104:ARG:HG2	1:B:2104:ARG:HH11	1.66	0.61
1:B:2498:LYS:HG2	1:B:2514:LEU:HD11	1.82	0.61
1:C:3364:MET:SD	3:C:3:NLX:C18	2.87	0.61
1:C:3478:ALA:N	1:C:3479:PRO:CD	2.63	0.61
1:C:3495:MET:HG3	1:C:3514:LEU:HD22	1.82	0.61
1:I:3352:LYS:HE3	1:I:3450:GLN:NE2	2.15	0.61
1:I:3447:TYR:C	1:I:3447:TYR:CD2	2.78	0.61
1:K:5258:LYS:HD2	1:K:5258:LYS:N	2.03	0.61
1:D:4309:GLN:NE2	1:D:4309:GLN:C	2.59	0.61
1:G:1355:PHE:CE1	1:G:1360:PRO:HG3	2.35	0.61
1:I:3363:LEU:HD13	4:I:7519:HOH:O	2.01	0.61
1:B:2024:PRO:HG3	1:B:2037:PHE:CZ	2.36	0.61
1:L:6024:PRO:HG3	1:L:6037: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:H:2086:MET:HE3	1:H:2112:LEU:HD21	1.83	0.61
1:A:1371:GLY:O	1:A:1414:LYS:HD3	2.00	0.60
1:C:3306:LEU:HD13	1:C:3364:MET:HE1	1.83	0.60
1:G:1452:ARG:HH11	1:G:1452:ARG:HG2	1.66	0.60
1:J:4023:PRO:HB2	1:J:4034:LEU:HD21	1.82	0.60
1:J:4302:LYS:NZ	1:J:4302:LYS:HB3	2.16	0.60
1:K:5366:TYR:HB3	1:K:5368:LEU:HD13	1.81	0.60
1:F:6417:PHE:O	1:F:6420:LEU:HB3	2.02	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:A:1257:LYS:HD2	1:A:1320:GLY:H	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1304:LEU:HB3	3:A:1:N LX:C20	2.31	0.60
1:E:5353:GLN:NE2	1:E:5465:ILE:H	1.99	0.60
1:F:6097:LEU:HD11	1:F:6101:PHE:CD2	2.36	0.60
1:F:6324:ASP:OD1	1:F:6326:MET:N	2.32	0.60
1:F:6350:ILE:C	1:F:6351:ASN:HD22	2.07	0.60
1:K:5304:LEU:HD22	3:K:5:N LX:C10	2.32	0.60
1:L:6478:ALA:HB3	1:L:6479:PRO:HD3	1.82	0.60
1:E:5266:GLU:O	1:E:5270:ILE:HG13	2.00	0.60
1:E:5452:ARG:NE	1:E:5462:LYS:HA	2.16	0.60
1:L:6104:ARG:HG2	1:L:6104:ARG:HH11	1.64	0.60
1:A:1145:MET:HB2	1:A:1304:LEU:HD21	1.83	0.60
1:A:1244:ILE:HG12	1:A:1347:MET:HB3	1.84	0.60
1:E:5330:LYS:HB3	1:E:5334:GLU:OE2	2.01	0.60
1:F:6355:PHE:CE1	1:F:6360:PRO:HG3	2.36	0.60
1:G:1064:ARG:NH1	1:G:1294:LEU:HD11	2.15	0.60
1:L:6428:VAL:HB	1:L:6429:PRO:HD3	1.83	0.60
1:E:5292:GLU:O	1:E:5296:GLU:HG3	2.02	0.60
1:F:6083:TYR:CE2	1:F:6108:ILE:HD13	2.37	0.60
1:G:1308:LEU:HD21	1:G:1367:PRO:CG	2.32	0.60
1:K:5487:GLU:O	1:K:5491:ARG:HG3	2.02	0.60
1:L:6086:MET:HG3	1:L:6112:LEU:HD23	1.82	0.60
1:L:6174:ILE:HG13	4:L:7009:HOH:O	2.01	0.60
1:E:5487:GLU:O	1:E:5491:ARG:HG3	2.01	0.60
1:I:3284:HIS:O	1:I:3288:GLN:HG2	2.02	0.60
1:I:3395:LEU:HB3	1:I:3550:LEU:HD11	1.84	0.60
1:H:2257:LYS:HE3	1:H:2316:GLN:HE22	1.66	0.60
1:I:3352:LYS:HG3	1:I:3353:GLN:HG3	1.82	0.60
1:J:4468:HIS:CD2	3:J:4:N LX:H21	2.36	0.60
1:K:5341:PHE:H	1:K:5341:PHE:HD2	1.50	0.60
1:L:6136:MET:HE1	1:L:6500:TRP:HB3	1.82	0.60
1:L:6538:LYS:HB3	1:L:6541:ASP:HB2	1.82	0.60
1:C:3332:PRO:O	1:C:3336:GLN:HG3	2.02	0.60
1:G:1268:ILE:HG12	1:G:1301:MET:HE2	1.82	0.60
1:H:2318:LEU:C	1:H:2318:LEU:HD12	2.25	0.60
1:H:2536:ALA:O	1:H:2537:GLN:HG3	2.01	0.60
1:L:6324:ASP:OD1	1:L:6326:MET:HB2	2.02	0.60
1:L:6409:ASP:HB3	1:L:6412:LYS:HB2	1.82	0.60
1:B:2402:LYS:HG2	1:B:2546:PHE:CE1	2.37	0.60
1:F:6136:MET:HB3	1:F:6218:PHE:CE1	2.37	0.60
1:F:6351:ASN:HB3	1:F:6466:GLY:O	2.02	0.60
1:I:3464:VAL:CG2	1:J:4370:GLU:HG3	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3083:TYR:CE2	1:C:3108:ILE:HD13	2.37	0.59
1:B:2216:THR:HG23	1:B:2242:ARG:CB	2.32	0.59
1:B:2255:LEU:HD23	1:B:2318:LEU:CD1	2.33	0.59
1:D:4025:VAL:HG22	1:D:4034:LEU:HD23	1.82	0.59
1:E:5104:ARG:HD2	4:E:7316:HOH:O	2.01	0.59
1:F:6029:VAL:HG13	4:F:7744:HOH:O	2.02	0.59
1:I:3364:MET:HE3	3:I:3:NLX:H201	1.84	0.59
1:K:5091:PRO:HG3	1:K:5112:LEU:HD21	1.84	0.59
1:L:6262:LYS:HB3	1:L:6263:PRO:HD3	1.82	0.59
1:A:1269:ALA:HB2	1:A:1282:MET:HE3	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:I:3180:THR:HG23	1:I:3185:SER:HB3	1.84	0.59
1:J:4134:PRO:HG2	1:J:4163:VAL:HG12	1.83	0.59
1:A:1359:ILE:HB	1:A:1360:PRO:HD3	1.84	0.59
1:A:1477:GLY:HA2	1:A:1493:SER:OG	2.03	0.59
1:B:2317:PRO:HB2	3:B:2:NLX:C19	2.31	0.59
1:I:3064:ARG:HD3	1:I:3065:PHE:CZ	2.37	0.59
1:I:3538:LYS:HE2	1:I:3541:ASP:OD1	2.02	0.59
1:L:6493:SER:O	1:L:6497:MET:HG3	2.01	0.59
1:B:2104:ARG:HG2	1:B:2104:ARG:NH1	2.17	0.59
1:B:2512:GLU:HB3	4:B:7018:HOH:O	2.01	0.59
1:C:3447:TYR:C	1:C:3447:TYR:CD2	2.79	0.59
1:D:4260:ASP:OD1	1:D:4262:LYS:HB3	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:A:1381:LEU:HD21	1:F:6459:MET:HB3	1.85	0.59
1:A:1421:ILE:CG2	1:A:1425:MET:HE2	2.32	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:I:3462:LYS:NZ	1:J:4376:LYS:NZ	2.50	0.59
1:K:5119:LEU:HD12	1:K:5119:LEU:O	2.02	0.59
1:L:6048:ALA:HB3	1:L:6123:THR:HG23	1.85	0.59
1:A:1478:ALA:N	1:A:1479:PRO:CD	2.65	0.59
1:D:4318:LEU:C	1:D:4318:LEU:HD12	2.28	0.59
1:F:6149:ALA:HB2	1:F:6169:GLN:HG3	1.84	0.59
1:I:3478:ALA:N	1:I:3479:PRO:CD	2.66	0.59
1:J:4027:ASP:OD1	1:J:4032:LYS:HD3	2.03	0.59
1:K:5395:LEU:HD21	1:K:5553:LYS:HB2	1.83	0.59
1:L:6233:SER:O	1:L:6342:HIS:NE2	2.34	0.59
1:C:3251:LEU:HD12	1:C:3433:VAL:HG23	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4038:VAL:HG21	1:D:4049:ILE:HD12	1.85	0.59
1:I:3526:TYR:CE2	1:I:3539:LEU:HB2	2.37	0.59
1:L:6086:MET:CE	1:L:6110:LEU:HB2	2.31	0.59
1:L:6420:LEU:CD1	1:L:6547:TRP:CZ2	2.85	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:F:6242:ARG:HG2	1:F:6242:ARG:NH1	2.15	0.59
1:F:6512:GLU:H	1:F:6512:GLU:CD	2.11	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: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:J:4304:LEU:HB3	3:J:4:NLX:H203	1.85	0.58
1:K:5447:TYR:HA	1:K:5527:LEU:O	2.03	0.58
1:L:6105:LYS:HD3	1:L:6106:GLU:CG	2.33	0.58
1:A:1309:GLN:NE2	1:A:1310:GLY:N	2.51	0.58
1:A:1333:GLU:H	1:A:1333:GLU:CD	2.11	0.58
1:C:3456:SER:HB3	1:C:3460:LYS:HD3	1.85	0.58
3:C:3:NLX:C20	3:C:3:NLX:C10	2.82	0.58
1:G:1313:ARG:HH11	1:G:1313:ARG:HG3	1.67	0.58
1:K:5339:ARG:HG3	1:K:5339:ARG:O	2.02	0.58
1:E:5491:ARG:HD2	4:E:7007:HOH:O	2.03	0.58
1:F:6132:ARG:HB3	1:F:6211:ASN:HB2	1.85	0.58
1:G:1218:PHE:HB3	1:G:1244:ILE:HB	1.84	0.58
1:H:2143:GLY:HA3	3:H:2:NLX:H152	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:3296:GLU:O	1:C:3300:LYS:HG3	2.04	0.58
1:C:3309:GLN:HG3	1:D:4096:LEU:HD13	1.83	0.58
1:C:3359:ILE:HB	1:C:3360:PRO:HD3	1.86	0.58
1:E:5048:ALA:HB3	1:E:5123:THR:HG23	1.84	0.58
1:G:1379:MET:SD	1:G:1397:PRO:HG3	2.44	0.58
1:K:5026:VAL:HG12	1:K:5027:ASP:N	2.17	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:B:2528:GLN:O	1:B:2533:THR:HA	2.04	0.58
1:C:3404:LEU:C	1:C:3406:GLY:H	2.11	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:6215:VAL:N	1:F:6241:HIS:HD2	1.99	0.58
1:J:4348:VAL:O	1:J:4446:MET:HA	2.04	0.58
1:D:4104:ARG:HD2	4:D:7709:HOH:O	2.01	0.58
1:D:4249:VAL:HB	1:D:4433:VAL:HG21	1.85	0.58
1:J:4220:GLU:HG3	1:J:4472:LEU:HD21	1.86	0.58
1:L:6264:LEU:HD22	1:L:6268:ILE:CD1	2.33	0.58
1:B:2359:ILE:CG1	3:B:2:N LX:H71	2.30	0.58
1:B:2390:CYS:HB3	4:B:7626:HOH:O	2.02	0.58
1:D:4262:LYS:HB3	1:D:4263:PRO:HD3	1.85	0.58
1:F:6334:GLU:O	1:F:6338:GLU:HG3	2.04	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:A:1319:LEU:HD12	1:A:1319:LEU:N	2.18	0.58
1:B:2040:LEU:HD13	1:B:2155:LEU:CD1	2.33	0.58
1:I:3318:LEU:HB2	4:I:7480:HOH:O	2.04	0.58
1:I:3462:LYS:HZ1	1:J:4376:LYS:NZ	1.98	0.58
1:K:5133:LEU:HD22	1:K:5162:ASN:O	2.04	0.58
1:L:6104:ARG:HG2	1:L:6104:ARG:NH1	2.19	0.58
1:F:6306:LEU:HD21	1:F:6384:LYS:O	2.04	0.58
1:G:1252:THR:O	1:G:1254:VAL:N	2.36	0.58
1:J:4126:ASP:OD1	1:J:4128:THR:HG23	2.04	0.58
1:L:6223:GLY:O	1:L:6227:VAL:HG23	2.04	0.58
1:C:3257:LYS:HE3	1:C:3322:VAL:CG1	2.33	0.57
1:F:6373:LEU:HD23	1:F:6414:LYS:HA	1.85	0.57
1:F:6435:ARG:O	1:F:6438:ARG:HB3	2.04	0.57
1:I:3456:SER:HB3	1:I:3460:LYS:HD3	1.84	0.57
1:J:4034:LEU:HD11	2:J:479:NAG:H82	1.86	0.57
1:A:1342:HIS:N	1:A:1342:HIS:CD2	2.70	0.57
1:C:3220:GLU:OE2	1:C:3221:SER:HB2	2.04	0.57
1:C:3318:LEU:HD21	3:C:3:N LX:H162	1.85	0.57
1:D:4301:MET:HG3	1:D:4303:PHE:CZ	2.39	0.57
1:E:5142:GLY:HA3	1:E:5146:VAL:O	2.04	0.57
1:E:5411:VAL:HA	4:E:7302:HOH:O	2.03	0.57
1:G:1308:LEU:HD21	1:G:1367:PRO:HG2	1.86	0.57
1:G:1521:ASN:HB2	1:G:1522:GLN:NE2	2.19	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:K:5025:VAL:HG22	1:K:5034:LEU:HD23	1.86	0.57
1:L:6140:HIS:HD2	1:L:6141:GLY:O	1.87	0.57
1:D:4363:LEU:HD22	3:D:4:N LX:H102	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1104:ARG:HH11	1:G:1104:ARG:CB	2.17	0.57
1:I:3364:MET:HG2	3:I:3:NLX:H201	1.85	0.57
1:I:3453:PRO:HD2	1:I:3470:ASP:OD2	2.04	0.57
1:J:4140:HIS:CD2	1:J:4147:GLY:HA3	2.40	0.57
1:J:4306:LEU:HD22	1:J:4366:TYR:CE1	2.39	0.57
1:K:5428:VAL:HG13	1:K:5544:VAL:HA	1.86	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:G:1495:MET:HE1	1:G:1533:THR:OG1	2.04	0.57
1:H:2215:VAL:H	1:H:2241:HIS:CD2	2.18	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: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:F:6024:PRO:HG3	1:F:6037:PHE:CZ	2.40	0.57
1:F:6095:GLN:O	1:F:6099:GLU:HG3	2.05	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:H:2371:GLY:CA	1:H:2414:LYS:HD3	2.35	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
1:F:6348:VAL:O	1:F:6446:MET:HA	2.04	0.57
1:C:3437:HIS:HD2	1:C:3444:THR:OG1	1.87	0.57
1:G:1371:GLY:O	1:G:1414:LYS:HD3	2.05	0.57
1:H:2370:GLU:C	1:H:2372:GLN:N	2.63	0.57
1:J:4349:GLY:HA3	1:J:4447:TYR:CZ	2.40	0.57
1:A:1140:HIS:HE1	4:A:7108:HOH:O	1.87	0.57
1:B:2220:GLU:OE2	1:B:2472:LEU:HD11	2.05	0.57
1:C:3421:ILE:HG22	1:C:3425:MET:HE2	1.86	0.57
1:C:3434:ALA:HB2	1:C:3446:MET:HE3	1.86	0.57
1:G:1527:LEU:HD11	1:G:1533:THR:HG22	1.87	0.57
1:L:6104:ARG:NE	1:L:6108:ILE:HD12	2.18	0.57
1:F:6467:ASP:N	1:F:6470:ASP:OD2	2.38	0.56
1:A:1132:ARG:HB3	1:A:1211:ASN:HB2	1.86	0.56
1:I:3229:VAL:HG13	1:I:3328:LEU:HD21	1.86	0.56
1:J:4404:LEU:HD23	1:J:4404:LEU:N	2.21	0.56
1:B:2215:VAL:H	1:B:2241:HIS:HD2	1.53	0.56
1:C:3138:TRP:CZ3	1:C:3219:GLY:HA2	2.39	0.56
1:C:3324:ASP:OD2	1:C:3327:LEU:HB3	2.05	0.56
1:C:3401:GLU:OE2	1:C:3405:GLY:HA3	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:5190:GLY:O	1:E:5194:GLN:HG3	2.05	0.56
1:E:5386:TYR:N	1:E:5387:PRO:HD2	2.20	0.56
1:F:6359:ILE:HG23	3:F:6:NLX:H152	1.87	0.56
1:H:2396:ILE:HB	1:H:2397:PRO:HD3	1.86	0.56
1:I:3242:ARG:HG2	1:I:3242:ARG:NH1	2.20	0.56
1:K:5138:TRP:CZ3	1:K:5219:GLY:HA2	2.40	0.56
1:K:5249:VAL:HB	1:K:5433:VAL:HG21	1.86	0.56
1:K:5367:PRO:C	1:K:5368:LEU:HD12	2.30	0.56
1:B:2132:ARG:HB3	1:B:2211:ASN:HB2	1.87	0.56
1:D:4335:LEU:O	1:D:4340:ASN:ND2	2.24	0.56
1:J:4215:VAL:N	1:J:4241:HIS:HD2	2.03	0.56
1:A:1304:LEU:CB	3:A:1:NLX:H203	2.34	0.56
1:E:5370:GLU:C	1:E:5372:GLN:H	2.13	0.56
1:E:5447:TYR:HA	1:E:5527:LEU:O	2.05	0.56
3:E:5:NLX:O4	3:E:5:NLX:H203	2.06	0.56
1:F:6359:ILE:HG12	3:F:6:NLX:H162	1.86	0.56
1:H:2370:GLU:HG3	1:K:5461:PRO:CG	2.35	0.56
1:I:3396:ILE:HB	1:I:3397:PRO:HD3	1.88	0.56
1:L:6357:TRP:O	1:L:6360:PRO:HD2	2.05	0.56
1:C:3237:LYS:HE2	1:C:3238:ASN:HD21	1.70	0.56
1:C:3332:PRO:HB2	1:C:3333:GLU:OE1	2.06	0.56
1:D:4057:LYS:HB3	1:D:4069:GLN:HB2	1.88	0.56
1:D:4311:ASP:HB3	1:D:4314:GLU:HG3	1.86	0.56
1:D:4420:LEU:C	1:D:4420:LEU:HD12	2.31	0.56
1:H:2304:LEU:HD13	3:H:2:NLX:H162	1.87	0.56
1:J:4223:GLY:O	1:J:4226:SER:HB2	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:A:1236:ALA:HA	1:A:1239:LEU:HD12	1.87	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:C:3234:PRO:O	1:C:3237:LYS:HG2	2.05	0.56
1:C:3359:ILE:HG23	3:C:3:NLX:H101	1.87	0.56
1:C:3532:ASN:HB3	1:C:3534:GLN:HE21	1.71	0.56
1:G:1104:ARG:NH1	1:G:1104:ARG:HB3	2.21	0.56
1:G:1371:GLY:C	1:G:1414:LYS:HD3	2.30	0.56
1:J:4107:ASN:HD22	1:J:4108:ILE:H	1.53	0.56
1:C:3144:LEU:HD13	1:C:3177:PHE:CE1	2.41	0.56
1:C:3350:ILE:O	1:C:3448:GLU:HA	2.06	0.56
1:G:1332:PRO:O	1:G:1336:GLN:HG2	2.05	0.56
1:G:1421:ILE:HG22	1:G:1425:MET:HE2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:3353:GLN:O	1:I:3467:ASP:HA	2.05	0.56
1:K:5039:SER:HB3	1:K:5046:PRO:HG3	1.87	0.56
1:B:2404:LEU:N	1:B:2404:LEU:HD23	2.21	0.56
1:C:3423:ASP:OD1	1:C:3540:LYS:HE3	2.06	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:A:1218:PHE:CB	1:A:1244:ILE:HB	2.36	0.56
1:J:4135:VAL:HB	1:J:4215:VAL:HG22	1.88	0.56
1:J:4371:GLY:O	1:J:4414:LYS:HD3	2.06	0.56
1:K:5355:PHE:HB2	1:K:5422:ALA:HB2	1.88	0.56
1:L:6093:ALA:HB1	3:L:6:NLX:H192	1.87	0.56
1:A:1027:ASP:OD2	1:A:1032:LYS:HG2	2.04	0.55
1:D:4265:ALA:HB1	1:D:4282:MET:HE1	1.88	0.55
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:B:2531:ALA:C	1:B:2532:ASN:HD22	2.13	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:F:6543:GLU:CD	1:F:6543:GLU:H	2.14	0.55
1:G:1097:LEU:HD11	1:G:1101:PHE:CE2	2.41	0.55
1:G:1350:ILE:C	1:G:1351:ASN:HD22	2.14	0.55
1:B:2297:THR:O	1:B:2301:MET:HG2	2.06	0.55
1:B:2385:SER:C	1:B:2387:PRO:HD2	2.32	0.55
1:I:3088:THR:CG2	1:I:3295:LEU:HD13	2.35	0.55
1:I:3257:LYS:HE2	1:I:3316:GLN:NE2	2.21	0.55
1:I:3353:GLN:HE22	1:I:3465:ILE:H	1.54	0.55
1:K:5122:TYR:HE2	4:K:7094:HOH:O	1.88	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:L:6456:SER:HB3	1:L:6460:LYS:HD3	1.89	0.55
1:A:1363:LEU:HB3	3:A:1:NLX:H91	1.87	0.55
1:C:3396:ILE:HB	1:C:3397:PRO:HD3	1.88	0.55
1:E:5309:GLN:HG2	1:E:5310:GLY:N	2.20	0.55
1:F:6447:TYR:C	1:F:6447:TYR:CD2	2.85	0.55
1:L:6420:LEU:HD12	1:L:6420:LEU:C	2.32	0.55
1:A:1396:ILE:HB	1:A:1397:PRO:HD3	1.89	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1392:ALA:O	1:A:1396:ILE:HG12	2.07	0.55
1:B:2468:HIS:CD2	3:B:2:N LX:O3	2.60	0.55
1:D:4447:TYR:C	1:D:4447:TYR:CD2	2.84	0.55
1:F:6447:TYR:HB3	1:F:6517:TRP:CZ2	2.41	0.55
1:H:2423:ASP:OD2	1:H:2543:GLU:HG2	2.07	0.55
1:I:3447:TYR:HB3	1:I:3517:TRP:HZ2	1.71	0.55
1:J:4237:LYS:HG2	1:J:4238:ASN:ND2	2.22	0.55
1:J:4343:THR:HB	1:J:4442:ALA:HB2	1.89	0.55
1:K:5234:PRO:O	1:K:5237:LYS:HG2	2.06	0.55
1:B:2262:LYS:O	1:B:2266:GLU:HG3	2.07	0.55
1:D:4421:ILE:HG22	1:D:4425:MET:CE	2.33	0.55
1:I:3095:GLN:HG2	1:J:4309:GLN:OE1	2.07	0.55
1:J:4304:LEU:CG	3:J:4:N LX:H203	2.34	0.55
1:L:6099:GLU:HG3	1:L:6107:ASN:OD1	2.07	0.55
1:L:6142:GLY:HA2	3:L:6:N LX:C8	2.36	0.55
1:A:1221:SER:HA	1:A:1247:SER:O	2.07	0.55
1:D:4478:ALA:N	1:D:4479:PRO:CD	2.70	0.55
1:I:3173:GLY:HA3	4:I:7644:HOH:O	2.06	0.55
1:L:6144:LEU:HB3	1:L:6177:PHE:CE2	2.41	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:1197:ALA:O	1:G:1201:VAL:HG23	2.07	0.55
1:G:1313:ARG:HA	1:G:1386:TYR:CD2	2.42	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:I:3249:VAL:HG23	1:I:3251:LEU:H	1.72	0.55
1:J:4331:THR:OG1	1:J:4334:GLU:HG3	2.07	0.55
1:E:5437:HIS:HD2	1:E:5444:THR:OG1	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:K:5220:GLU:HG2	1:K:5472:LEU:HD21	1.90	0.54
1:K:5370:GLU:C	1:K:5372:GLN:H	2.15	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:H:2223:GLY:O	1:H:2227:VAL:HG23	2.07	0.54
1:H:2258:LYS:HD2	1:H:2258:LYS:H	1.70	0.54
1:D:4145:MET:HG3	1:D:4304:LEU:CD1	2.37	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:6524:GLU:OE2	1:L:6538:LYS:HG2	2.06	0.54
1:I:3119:LEU:HD12	1:I:3119:LEU:O	2.06	0.54
1:K:5022:SER:N	4:K:7180:HOH:O	2.40	0.54
1:K:5086:MET:HE3	1:K:5089:GLN:NE2	2.22	0.54
1:C:3329:LEU:HG	4:C:7056:HOH:O	2.06	0.54
1:E:5313:ARG:HG2	1:E:5386:TYR:CE2	2.43	0.54
1:G:1313:ARG:HG2	1:G:1386:TYR:CE2	2.42	0.54
1:K:5112:LEU:HD12	1:K:5112:LEU:N	2.23	0.54
1:E:5105:LYS:HE2	1:E:5483:GLU:HG3	1.88	0.54
1:I:3491:ARG:NH1	1:I:3491:ARG:HB3	2.22	0.54
1:K:5149:ALA:CB	1:K:5169:GLN:HG3	2.38	0.54
1:K:5221:SER:O	1:K:5225:GLU:N	2.37	0.54
1:K:5505:ARG:NH1	4:K:7766:HOH:O	2.40	0.54
1:L:6395:LEU:HD22	1:L:6550:LEU:CD1	2.37	0.54
1:B:2237:LYS:HB2	4:B:7015:HOH:O	2.07	0.54
1:D:4244:ILE:HG12	1:D:4347:MET:HB3	1.90	0.54
1:F:6414:LYS:HD2	1:F:6414:LYS:C	2.32	0.54
1:I:3243:ALA:O	1:I:3346:TYR:HA	2.07	0.54
1:J:4420:LEU:CD1	1:J:4547:TRP:HZ2	2.21	0.54
1:K:5079:ASN:ND2	2:K:579:NAG:C1	2.71	0.54
1:C:3089:GLN:OE1	1:C:3146:VAL:HB	2.07	0.54
1:D:4124:PRO:HD3	1:D:4158:ALA:HB1	1.89	0.54
1:D:4215:VAL:H	1:D:4241:HIS:CD2	2.07	0.54
1:E:5333:GLU:OE1	1:E:5333:GLU:N	2.33	0.54
1:F:6540:LYS:HA	1:F:6543:GLU:OE1	2.08	0.54
1:H:2363:LEU:CD1	3:H:2:NLX:H101	2.36	0.54
1:I:3278:THR:OG1	1:I:3281:VAL:HG23	2.07	0.54
1:L:6105:LYS:CD	1:L:6106:GLU:HG3	2.37	0.54
1:G:1304:LEU:CD1	1:G:1318:LEU:HB3	2.38	0.54
1:H:2316:GLN:OE1	1:H:2317:PRO:HD2	2.07	0.54
1:F:6257:LYS:HB2	1:F:6322:VAL:HG12	1.90	0.54
1:F:6264:LEU:O	1:F:6264:LEU:HD22	2.07	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:I:3420:LEU:HD13	1:I:3547:TRP:CZ2	2.43	0.54
1:J:4456:SER:HB3	1:J:4460:LYS:HD3	1.90	0.54
1:A:1079:ASN:HD22	2:A:179:NAG:H2	1.74	0.53
1:A:1131:ASN:O	1:A:1132:ARG:HG2	2.07	0.53
1:A:1134:PRO:CG	1:A:1163:VAL:HG12	2.32	0.53
1:C:3404:LEU:O	1:C:3406:GLY:N	2.41	0.53
1:K:5394:GLU:HG3	1:K:5395:LEU:HG	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:6177:PHE:HB2	1:L:6319:LEU:HD22	1.90	0.53
1:A:1318:LEU:HD12	1:A:1318:LEU:O	2.08	0.53
1:D:4091:PRO:HB3	1:D:4112:LEU:HD11	1.90	0.53
1:D:4386:TYR:N	1:D:4387:PRO:HD2	2.23	0.53
1:G:1092:LYS:HZ2	1:L:6302:LYS:HB2	1.73	0.53
1:H:2456:SER:HB2	1:H:2460:LYS:CD	2.39	0.53
1:I:3428:VAL:O	1:I:3432:ILE:HG13	2.08	0.53
1:J:4264:LEU:CD1	1:J:4316:GLN:HG2	2.38	0.53
1:C:3370:GLU:HG3	1:D:4461:PRO:CG	2.39	0.53
1:D:4132:ARG:HB3	1:D:4211:ASN:HB2	1.91	0.53
1:G:1435:ARG:HH12	1:G:1544:VAL:HG11	1.73	0.53
1:H:2540:LYS:O	1:H:2544:VAL:HG23	2.09	0.53
1:K:5357:TRP:O	1:K:5361:MET:HB2	2.08	0.53
1:L:6358:LEU:HG	1:L:6363:LEU:CD1	2.38	0.53
1:A:1260:ASP:OD2	1:A:1263:PRO:HD3	2.08	0.53
1:F:6271:THR:HG22	1:F:6297:THR:HG23	1.90	0.53
1:G:1026:VAL:CG1	1:G:1027:ASP:N	2.71	0.53
1:G:1132:ARG:HB3	1:G:1211:ASN:HB2	1.89	0.53
1:H:2104:ARG:HG2	1:H:2104:ARG:HH11	1.73	0.53
1:H:2216:THR:HG23	1:H:2242:ARG:HB2	1.90	0.53
1:I:3217:ILE:CD1	1:I:3227:VAL:HG13	2.38	0.53
1:L:6359:ILE:HD11	1:L:6468:HIS:ND1	2.23	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: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:L:6130:LYS:HE3	1:L:6130:LYS:H	1.74	0.53
1:A:1392:ALA:HB1	1:A:1394:GLU:OE2	2.08	0.53
1:B:2112:LEU:O	1:B:2113:SER:HB2	2.07	0.53
1:D:4131:ASN:O	1:D:4132:ARG:NH1	2.42	0.53
1:D:4251:LEU:CD2	1:D:4333:GLU:HG3	2.39	0.53
1:F:6537:GLN:O	1:F:6538:LYS:HB2	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:A:1289:LYS:HA	1:A:1293:GLU:OE2	2.08	0.53
1:A:1539:LEU:HG	1:A:1540:LYS:HG2	1.89	0.53
1:B:2083:TYR:CZ	1:B:2108:ILE:HD13	2.43	0.53
1:B:2095:GLN:O	1:B:2099:GLU:HG3	2.08	0.53
1:B:2318:LEU:HG	3:B:2:N LX:C17	2.36	0.53
1:D:4353:GLN:O	1:D:4467:ASP:HA	2.09	0.53
1:G:1087:CYS:O	1:G:1088:THR:C	2.51	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1552:ALA:O	1:G:1553:LYS:HB2	2.07	0.53
1:J:4551:PHE:C	1:J:4553:LYS:H	2.16	0.53
1:B:2043:PHE:HB3	4:B:7515:HOH:O	2.08	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:F:6026:VAL:CG1	1:F:6207:SER:HB3	2.39	0.53
1:F:6097:LEU:HB2	3:F:6:N LX:C19	2.39	0.53
1:G:1349:GLY:HA3	1:G:1447:TYR:CE1	2.43	0.53
1:G:1404:LEU:HB3	1:G:1413:LYS:CG	2.39	0.53
1:H:2355:PHE:CE1	1:H:2360:PRO:HB3	2.43	0.53
1:J:4079:ASN:CG	2:J:479:NAG:C1	2.82	0.53
1:L:6324:ASP:OD1	1:L:6326:MET:N	2.39	0.53
1:C:3302:LYS:HD2	1:D:4092:LYS:HD3	1.90	0.53
1:I:3348:VAL:O	1:I:3446:MET:HA	2.08	0.53
1:I:3357:TRP:O	1:I:3360:PRO:HD2	2.09	0.53
1:J:4313:ARG:HD3	1:J:4383:TRP:HH2	1.74	0.53
1:L:6417:PHE:O	1:L:6420:LEU:HB3	2.08	0.53
1:C:3382:LEU:HD11	1:C:3420:LEU:HD11	1.90	0.53
1:G:1304:LEU:HD11	1:G:1318:LEU:HD23	1.89	0.53
1:H:2306:LEU:HD22	1:H:2366:TYR:CE1	2.44	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:L:6235:LEU:HD12	1:L:6327:LEU:CD1	2.32	0.53
1:B:2149:ALA:CB	1:B:2169:GLN:HG3	2.39	0.52
3:D:4:N LX:O2	4:D:7001:HOH:O	2.19	0.52
1:E:5140:HIS:CD2	1:E:5147:GLY:HA3	2.44	0.52
1:E:5308:LEU:HD21	1:E:5367:PRO:HG2	1.90	0.52
1:F:6359:ILE:HA	3:F:6:N LX:H162	1.91	0.52
1:G:1026:VAL:HG12	1:G:1027:ASP:N	2.24	0.52
1:H:2350:ILE:HD12	1:H:2350:ILE:O	2.09	0.52
3:H:2:N LX:H203	3:H:2:N LX:O4	2.09	0.52
1:J:4132:ARG:HH12	1:J:4206:ALA:HB2	1.73	0.52
1:K:5342:HIS:HA	4:K:7948:HOH:O	2.08	0.52
1:C:3092:LYS:CD	1:D:4302:LYS:HD2	2.39	0.52
1:D:4266:GLU:O	1:D:4270:ILE:HG13	2.08	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:H:2107:ASN:ND2	1:H:2108:ILE:H	2.07	0.52
1:I:3250:ALA:O	1:I:3256:VAL:HG21	2.08	0.52
1:K:5550:LEU:HD23	1:K:5550:LEU:C	2.34	0.52
1:B:2103:ASN:ND2	1:B:2481:LEU:HD12	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2420:LEU:C	1:B:2420:LEU:HD12	2.34	0.52
1:G:1218:PHE:HB2	1:G:1244:ILE:HB	1.91	0.52
1:H:2097:LEU:HD11	1:H:2101:PHE:CE2	2.45	0.52
1:I:3386:TYR:O	1:I:3390:CYS:N	2.40	0.52
1:K:5465:ILE:HD12	1:K:5465:ILE:N	2.24	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:C:3286:LEU:HA	1:C:3289:LYS:HG2	1.92	0.52
1:E:5348:VAL:O	1:E:5446:MET:HA	2.09	0.52
1:F:6258:LYS:H	1:F:6258:LYS:CE	2.21	0.52
1:G:1348:VAL:O	1:G:1446:MET:HA	2.10	0.52
1:H:2260:ASP:OD1	1:H:2263:PRO:HD3	2.10	0.52
1:K:5370:GLU:O	1:K:5372:GLN:HG3	2.10	0.52
1:L:6023:PRO:HB2	1:L:6034:LEU:CD2	2.38	0.52
1:D:4089:GLN:OE1	1:D:4146:VAL:HB	2.10	0.52
1:E:5140:HIS:HD2	1:E:5141:GLY:O	1.92	0.52
1:E:5252:THR:HG22	1:E:5252:THR:O	2.08	0.52
1:G:1221:SER:HB2	3:G:1:N LX:O1	2.10	0.52
1:G:1452:ARG:HG2	1:G:1452:ARG:NH1	2.24	0.52
1:H:2228:SER:CB	1:H:2250:ALA:H	2.23	0.52
1:L:6526:TYR:HE1	1:L:6528:GLN:HG2	1.74	0.52
1:L:6533:THR:O	1:L:6534:GLN:HG3	2.10	0.52
1:E:5404:LEU:CD2	1:E:5416:LEU:HB2	2.40	0.52
1:E:5538:LYS:O	1:E:5541:ASP:HB2	2.08	0.52
1:I:3026:VAL:HG12	1:I:3027:ASP:N	2.24	0.52
1:I:3152:TYR:N	1:I:3152:TYR:CD1	2.77	0.52
1:I:3432:ILE:O	1:I:3435:ARG:HB2	2.09	0.52
1:J:4482:LYS:HE2	4:J:7544:HOH:O	2.07	0.52
1:K:5223:GLY:O	1:K:5227:VAL:HG23	2.10	0.52
1:L:6225:GLU:HG3	1:L:6255:LEU:HD13	1.91	0.52
1:L:6290:THR:OG1	1:L:6293:GLU:HG3	2.09	0.52
1:A:1133:LEU:HB3	1:A:1134:PRO:HD2	1.91	0.52
1:B:2396:ILE:HB	1:B:2397:PRO:HD3	1.91	0.52
1:C:3436:ASN:HD22	1:C:3436:ASN:N	2.08	0.52
1:F:6097:LEU:HD13	3:F:6:N LX:C19	2.40	0.52
1:F:6395:LEU:HD13	1:F:6550:LEU:HD23	1.91	0.52
1:I:3215:VAL:H	1:I:3241:HIS:CD2	2.25	0.52
1:K:5428:VAL:O	1:K:5432:ILE:HG13	2.09	0.52
1:E:5297:THR:O	1:E:5301:MET:HG2	2.10	0.52
1:E:5428:VAL:O	1:E:5429:PRO:C	2.50	0.52
1:H:2371:GLY:HA2	1:H:2414:LYS:CD	2.37	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:4079:ASN:ND2	2:J:479:NAG:C5	2.72	0.52
1:J:4431:VAL:HG21	1:J:4540:LYS:HB2	1.92	0.52
1:K:5186:ARG:HB3	1:K:5324:ASP:HB2	1.91	0.52
1:K:5346:TYR:HB3	1:K:5437:HIS:CD2	2.45	0.52
1:A:1351:ASN:ND2	1:A:1449:PHE:HB3	2.25	0.52
1:A:1498:LYS:CD	1:A:1514:LEU:HD11	2.30	0.52
1:B:2340:ASN:HB3	4:B:7205:HOH:O	2.08	0.52
1:D:4235:LEU:HD12	1:D:4327:LEU:HD12	1.90	0.52
1:I:3389:VAL:HB	1:I:3424:VAL:HG11	1.92	0.52
1:I:3490:ILE:O	1:I:3494:LYS:HG3	2.10	0.52
1:J:4100:LEU:O	1:J:4101:PHE:HD1	1.93	0.52
1:J:4104:ARG:NH2	1:J:4150:SER:O	2.40	0.52
1:J:4252:THR:O	1:J:4254:VAL:N	2.43	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: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:G:1399:ALA:HB2	1:G:1550:LEU:CD2	2.40	0.52
1:I:3407:THR:HG21	1:I:3412:LYS:HD3	1.92	0.52
1:K:5392:ALA:O	1:K:5396:ILE:HG12	2.09	0.52
1:A:1374:ASP:O	1:A:1375:GLN:C	2.54	0.51
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: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:H:2459:MET:SD	1:K:5308:LEU:HD22	2.50	0.51
1:I:3330:LYS:HG3	1:I:3335:LEU:HD21	1.92	0.51
1:A:1402:LYS:HG3	1:A:1402:LYS:O	2.10	0.51
1:B:2359:ILE:HG23	3:B:2:NLX:C7	2.40	0.51
1:C:3186:ARG:HB3	1:C:3324:ASP:HB2	1.91	0.51
1:E:5079:ASN:HD21	2:E:579:NAG:C1	2.22	0.51
1:F:6107:ASN:HD22	1:F:6108:ILE:N	2.07	0.51
1:F:6359:ILE:HG12	3:F:6:NLX:H151	1.91	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:B:2359:ILE:HD13	3:B:2:NLX:H72	1.91	0.51
1:C:3104:ARG:O	1:C:3482:LYS:HE3	2.09	0.51
1:C:3371:GLY:O	1:C:3411:VAL:HG13	2.10	0.51
1:E:5363:LEU:HD13	3:E:5:NLX:H203	1.91	0.51
1:E:5491:ARG:HG2	1:E:5491:ARG:HH11	1.74	0.51
1:H:2501:ALA:O	1:H:2505:ARG:HG2	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:4230:LEU:O	1:J:4342:HIS:HE1	1.93	0.51
1:K:5057:LYS:HG3	1:K:5058:PRO:HD2	1.92	0.51
1:L:6188:ASN:ND2	1:L:6327:LEU:HD23	2.25	0.51
1:L:6304:LEU:CD2	3:L:6:N LX:H102	2.38	0.51
1:L:6410:THR:HA	1:L:6413:LYS:HG3	1.91	0.51
1:B:2527:LEU:HD11	1:B:2533:THR:HG22	1.93	0.51
1:E:5105:LYS:HZ3	1:E:5482:LYS:HA	1.75	0.51
1:E:5220:GLU:HG3	4:E:7086:HOH:O	2.11	0.51
1:I:3386:TYR:N	1:I:3387:PRO:HD2	2.25	0.51
1:K:5110:LEU:HD11	1:K:5150:SER:HB2	1.92	0.51
1:A:1188:ASN:O	1:A:1189:TRP:C	2.53	0.51
1:A:1215:VAL:N	1:A:1241:HIS:HD2	1.96	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:D:4355:PHE:CE2	1:D:4425:MET:HE1	2.45	0.51
1:E:5203:ASP:N	1:E:5203:ASP:OD1	2.42	0.51
1:F:6426:PHE:O	1:F:6429:PRO:HD2	2.10	0.51
1:H:2343:THR:HB	1:H:2442:ALA:HB2	1.92	0.51
1:A:1124:PRO:HD3	1:A:1158:ALA:HB1	1.92	0.51
1:A:1304:LEU:CG	3:A:1:N LX:H203	2.40	0.51
1:D:4427:GLY:O	1:D:4431:VAL:HG23	2.11	0.51
1:F:6142:GLY:C	3:F:6:N LX:H82	2.36	0.51
1:F:6214:SER:HA	1:F:6241:HIS:CD2	2.45	0.51
1:G:1120:ASN:HB2	1:G:1167:THR:OG1	2.11	0.51
1:G:1339:ARG:NH1	1:G:1436:ASN:HD22	2.09	0.51
1:I:3139:ILE:HG12	1:I:3168:ILE:HD11	1.91	0.51
1:I:3431:VAL:HG21	1:I:3540:LYS:HB2	1.93	0.51
1:J:4174:ILE:HA	1:J:4319:LEU:HD12	1.92	0.51
1:J:4235:LEU:HD12	1:J:4327:LEU:HD12	1.92	0.51
1:J:4313:ARG:HA	1:J:4386:TYR:CD2	2.45	0.51
1:J:4542:LYS:HB2	4:J:7954:HOH:O	2.09	0.51
1:K:5063:LEU:O	1:K:5066:THR:HG23	2.11	0.51
1:A:1104:ARG:HH11	1:A:1104:ARG:HG2	1.74	0.51
1:B:2493:SER:O	1:B:2497:MET:HG3	2.11	0.51
1:C:3333:GLU:OE1	1:C:3333:GLU:N	2.43	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:E:5318:LEU:HD11	3:E:5:N LX:H11	1.92	0.51
1:E:5354:GLU:OE1	1:E:5354:GLU:HA	2.11	0.51
1:H:2350:ILE:HD12	1:H:2350:ILE:C	2.35	0.51
1:K:5217:ILE:CD1	1:K:5227:VAL:HG13	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:5126:ASP:H	1:E:5131:ASN:HD21	1.56	0.51
1:E:5478:ALA:N	1:E:5479:PRO:CD	2.74	0.51
1:F:6025:VAL:HG22	1:F:6034:LEU:HD23	1.92	0.51
1:I:3029:VAL:HG23	1:I:3204:ASN:OD1	2.11	0.51
1:A:1435:ARG:O	1:A:1438:ARG:HB3	2.11	0.51
1:B:2179:SER:O	1:B:2265:ALA:HB2	2.11	0.51
1:G:1334:GLU:O	1:G:1338:GLU:HG2	2.11	0.51
1:H:2104:ARG:HG2	1:H:2104:ARG:NH1	2.26	0.51
1:H:2176:GLY:CA	1:H:2189:TRP:HB2	2.38	0.51
1:H:2241:HIS:C	1:H:2242:ARG:HD2	2.36	0.51
1:H:2252:THR:O	1:H:2252:THR:HG22	2.11	0.51
1:I:3236:ALA:O	1:I:3239:LEU:HB2	2.11	0.51
1:I:3364:MET:SD	3:I:3:NLX:H201	2.50	0.51
1:I:3400:THR:HG23	1:I:3404:LEU:HD12	1.92	0.51
1:L:6444:THR:HG22	1:L:6520:TYR:HB3	1.92	0.51
1:A:1364:MET:HG3	3:A:1:NLX:H82	1.92	0.51
1:A:1486:SER:O	1:A:1490:ILE:HG13	2.11	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:G:1079:ASN:CG	2:G:179:NAG:C1	2.84	0.51
1:H:2268:ILE:HD11	1:H:2319:LEU:HD21	1.91	0.51
1:H:2492:LEU:O	1:H:2496:VAL:HG23	2.11	0.51
1:I:3338:GLU:HB2	1:I:3340:ASN:HB2	1.93	0.51
1:K:5371:GLY:CA	1:K:5414:LYS:HD3	2.37	0.51
1:K:5550:LEU:C	1:K:5552:ALA:H	2.18	0.51
1:A:1045:GLN:HB2	1:L:6486:SER:HA	1.93	0.50
1:A:1431:VAL:HG11	1:A:1544:VAL:HG21	1.92	0.50
1:C:3329:LEU:C	1:C:3330:LYS:HG2	2.36	0.50
1:E:5220:GLU:HG2	1:E:5472:LEU:HD21	1.92	0.50
1:G:1526:TYR:CD2	1:G:1539:LEU:HB2	2.45	0.50
1:I:3244:ILE:HG23	1:I:3347:MET:HB3	1.92	0.50
1:J:4508:ASN:OD1	1:J:4510:ASN:HB2	2.11	0.50
1:K:5393:LYS:HA	1:K:5396:ILE:CG1	2.41	0.50
1:K:5429:PRO:O	1:K:5433:VAL:HG23	2.11	0.50
1:D:4171:ARG:O	1:D:4176:GLY:HA3	2.11	0.50
1:G:1152:TYR:N	1:G:1152:TYR:CD1	2.79	0.50
1:H:2097:LEU:HD11	3:H:2:NLX: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:L:6452:ARG:HD2	1:L:6464:VAL:O	2.11	0.50
1:B:2359:ILE:CG1	3:B:2:NLX:C7	2.85	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3143:GLY:CA	3:C:3:NLX:H152	2.34	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:I:3125:ALA:HB1	1:I:3131:ASN:ND2	2.25	0.50
1:I:3268:ILE:CG1	1:I:3301:MET:HE2	2.40	0.50
1:I:3467:ASP:OD1	1:I:3468:HIS:N	2.41	0.50
1:J:4221:SER:OG	3:J:4:NLX:O1	2.28	0.50
1:J:4262:LYS:HB3	1:J:4263:PRO:HD3	1.92	0.50
1:J:4332:PRO:O	1:J:4336:GLN:HG2	2.11	0.50
1:J:4363:LEU:HD22	3:J:4:NLX:H192	1.93	0.50
1:J:4532:ASN:HB2	4:J:7463:HOH:O	2.10	0.50
1:L:6386:TYR:N	1:L:6387:PRO:HD2	2.27	0.50
1:C:3143:GLY:HA2	3:C:3:NLX:H51	1.94	0.50
1:D:4101:PHE:CE2	3:D:4:NLX:H21	2.46	0.50
1:E:5372:GLN:HB3	4:E:7425:HOH:O	2.11	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:I:3223:GLY:O	1:I:3227:VAL:HG23	2.10	0.50
1:I:3526:TYR:CD2	1:I:3539:LEU:HB2	2.46	0.50
1:L:6225:GLU:HG3	1:L:6255:LEU:CD1	2.42	0.50
1:A:1498:LYS:HD3	1:A:1502:ASN:HD21	1.76	0.50
1:C:3425:MET:HE3	1:C:3426:PHE:HE1	1.77	0.50
1:D:4121:ILE:HG12	1:D:4166:VAL:HG22	1.94	0.50
1:D:4543:GLU:OE2	1:D:4543:GLU:N	2.31	0.50
1:E:5527:LEU:HD11	1:E:5533:THR:HG22	1.92	0.50
1:F:6161:GLU:HG3	1:F:6501:ALA:HB2	1.93	0.50
1:G:1244:ILE:HD11	1:G:1503:PHE:HD2	1.76	0.50
1:I:3252:THR:HG23	1:I:3425:MET:O	2.12	0.50
1:I:3404:LEU:HD22	1:I:3413:LYS:O	2.10	0.50
1:J:4363:LEU:HD22	3:J:4:NLX:H181	1.92	0.50
1:K:5246:GLU:O	1:K:5247:SER:HB2	2.10	0.50
1:K:5363:LEU:HB3	3:K:5:NLX:H201	1.93	0.50
1:K:5517:TRP:CE3	1:K:5527:LEU:HD23	2.47	0.50
1:K:5524:GLU:O	1:K:5537:GLN:O	2.29	0.50
1:C:3104:ARG:CZ	1:C:3153:ASP:HB2	2.41	0.50
1:E:5079:ASN:ND2	2:E:579:NAG:C1	2.75	0.50
1:E:5412:LYS:O	1:E:5416:LEU:HG	2.11	0.50
1:F:6428:VAL:HG21	1:F:6547:TRP:CD1	2.47	0.50
1:G:1265:ALA:HB1	1:G:1282:MET:HE1	1.94	0.50
1:I:3103:ASN:ND2	1:I:3481:LEU:HD12	2.25	0.50
1:I:3330:LYS:HG3	1:I:3335:LEU:CD2	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:5161:GLU:CD	1:K:5498:LYS:HA	2.36	0.50
1:L:6149:ALA:HB2	1:L:6169:GLN:HG3	1.94	0.50
1:H:2144:LEU:HD22	1:H:2177:PHE:CZ	2.46	0.50
1:I:3038:VAL:HG12	1:I:3039:SER:N	2.26	0.50
1:I:3218:PHE:HA	1:I:3244:ILE:O	2.12	0.50
1:J:4452:ARG:HD2	1:J:4464:VAL:O	2.12	0.50
3:K:5:N LX:H203	3:K:5:N LX:O4	2.12	0.50
1:A:1463:THR:HG21	1:F:6372:GLN:CB	2.41	0.50
1:D:4480:PHE:O	1:D:4481:LEU:HD23	2.12	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:I:3317:PRO:C	3:I:3:N LX:H192	2.36	0.50
1:J:4526:TYR:CE1	1:J:4539:LEU:HD13	2.46	0.50
1:K:5264:LEU:HD21	1:K:5319:LEU:HD23	1.94	0.50
1:C:3420:LEU:C	1:C:3420:LEU:HD12	2.37	0.50
1:D:4126:ASP:OD2	1:D:4129:LYS:HG3	2.12	0.50
1:E:5158:ALA:O	1:E:5162:ASN:HA	2.11	0.50
1:F:6242:ARG:HD3	1:F:6503:PHE:O	2.12	0.50
1:F:6252:THR:HG22	1:F:6254:VAL:HG12	1.93	0.50
1:G:1260:ASP:O	1:G:1263:PRO:HD2	2.12	0.50
1:G:1383:TRP:CZ3	1:G:1393:LYS:HB2	2.47	0.50
1:H:2453:PRO:C	1:H:2455:PHE:H	2.18	0.50
1:I:3134:PRO:HG2	1:I:3163:VAL:HG12	1.94	0.50
1:I:3257:LYS:NZ	1:I:3316:GLN:CG	2.75	0.50
1:I:3309:GLN:HG3	1:J:4095:GLN:NE2	2.27	0.50
1:I:3480:PHE:CE1	1:I:3497:MET:HE1	2.47	0.50
1:K:5271:THR:HG22	1:K:5297:THR:HG23	1.94	0.50
1:A:1233:SER:OG	1:A:1327:LEU:HD12	2.12	0.49
1:B:2053:ILE:HD12	1:B:2121:ILE:HD12	1.94	0.49
1:D:4201:VAL:HG13	1:D:4205:ILE:HB	1.94	0.49
1:E:5135:VAL:HG21	1:E:5205:ILE:HG21	1.93	0.49
1:F:6186:ARG:HB3	1:F:6324:ASP:HB2	1.94	0.49
1:F:6426:PHE:C	1:F:6429:PRO:HD2	2.37	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:J:4074:TRP:CD2	1:J:4078:LYS:HE2	2.47	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:L:6143:GLY:HA3	3:L:6:N LX:H11	1.94	0.49
1:L:6260:ASP:O	1:L:6263:PRO:HD2	2.12	0.49
1:L:6545:ALA:HA	1:L:6548:THR:HG22	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1348:VAL:O	1:A:1446:MET:HA	2.11	0.49
1:B:2024:PRO:O	1:B:2034:LEU:HD23	2.12	0.49
1:I:3079:ASN:OD1	2:I:379:NAG:C1	2.60	0.49
1:K:5540:LYS:O	1:K:5544:VAL:HG23	2.13	0.49
1:L:6414:LYS:HD2	1:L:6414:LYS:C	2.37	0.49
1:L:6420:LEU:HD11	1:L:6547:TRP:CZ2	2.46	0.49
1:A:1145:MET:HB2	1:A:1304:LEU:CD2	2.42	0.49
1:A:1297:THR:O	1:A:1301:MET:HG2	2.12	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:E:5371:GLY:C	1:E:5414:LYS:HD3	2.37	0.49
1:G:1268:ILE:CG1	1:G:1301:MET:HE2	2.42	0.49
1:G:1283:VAL:O	1:G:1287:ARG:HG3	2.12	0.49
1:I:3275:LYS:HG3	4:I:7145:HOH:O	2.11	0.49
1:J:4119:LEU:HD12	1:J:4119:LEU:O	2.12	0.49
1:L:6317:PRO:HG3	1:L:6387:PRO:HB2	1.94	0.49
1:A:1105:LYS:HD2	1:A:1483:GLU:OE2	2.12	0.49
1:A:1382:LEU:HD22	1:A:1420:LEU:HD21	1.93	0.49
1:C:3070:PRO:HG2	4:C:7964:HOH:O	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:I:3218:PHE:CB	1:I:3244:ILE:HB	2.43	0.49
1:K:5351:ASN:ND2	1:K:5449:PHE:HB3	2.27	0.49
1:L:6138:TRP:HA	1:L:6218:PHE:O	2.12	0.49
1:A:1302:LYS:HG3	4:A:7839:HOH:O	2.12	0.49
1:B:2478:ALA:HB3	1:B:2479:PRO:HD3	1.93	0.49
1:C:3304:LEU:HD22	3:C:3:NLX:H201	1.95	0.49
1:F:6090:ASP:HB3	1:F:6093:ALA:HB3	1.93	0.49
1:H:2359:ILE:CD1	3:H:2:NLX:H71	2.39	0.49
1:I:3431:VAL:HG22	1:I:3446:MET:HE1	1.94	0.49
1:J:4414:LYS:O	1:J:4418:LEU:HG	2.12	0.49
1:K:5258:LYS:H	1:K:5258:LYS:CD	2.06	0.49
1:K:5304:LEU:HD13	3:K:5:NLX:C18	2.37	0.49
1:K:5311:ASP:OD1	1:K:5313:ARG:HB2	2.12	0.49
1:K:5333:GLU:H	1:K:5333:GLU:CD	2.19	0.49
1:L:6304:LEU:HD13	3:L:6:NLX:C18	2.41	0.49
1:L:6471:GLU:O	1:L:6475:VAL:HG23	2.12	0.49
1:A:1034:LEU:HD13	1:A:1034:LEU:C	2.38	0.49
1:A:1350:ILE:O	1:A:1448:GLU:HA	2.12	0.49
1:B:2355:PHE:CD2	1:B:2359:ILE:HG21	2.48	0.49
1:C:3313:ARG:HG2	1:C:3386:TYR:CZ	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:2057:LYS:HD2	4:H:7830:HOH:O	2.12	0.49
1:H:2103:ASN:ND2	1:H:2481:LEU:HD12	2.28	0.49
1:H:2264:LEU:HD21	1:H:2319:LEU:HD23	1.95	0.49
1:J:4244:ILE:HG12	1:J:4347:MET:HB3	1.94	0.49
1:J:4359:ILE:HG23	3:J:4:N LX:C8	2.43	0.49
1:L:6198:LEU:HD21	1:L:6217:ILE:CG2	2.42	0.49
1:C:3308:LEU:HG	4:C:7642:HOH:O	2.11	0.49
1:C:3364:MET:CE	3:C:3:N LX:C18	2.73	0.49
1:D:4309:GLN:C	1:D:4309:GLN:HE21	2.20	0.49
1:D:4335:LEU:HD11	4:D:7303:HOH:O	2.12	0.49
1:E:5086:MET:HE2	1:E:5112:LEU:HD21	1.94	0.49
1:G:1468:HIS:NE2	3:G:1:N LX:O1	2.46	0.49
1:H:2304:LEU:HD22	3:H:2:N LX:C20	2.42	0.49
1:H:2348:VAL:O	1:H:2446:MET:HA	2.12	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:I:3229:VAL:HG11	1:I:3327:LEU:HD21	1.94	0.49
1:J:4473:PHE:HA	4:J:7950:HOH:O	2.11	0.49
1:J:4525:GLY:CA	1:J:4537:GLN:HG2	2.42	0.49
1:K:5060:LEU:CD2	1:K:5114:GLU:HB2	2.43	0.49
1:K:5393:LYS:HA	1:K:5396:ILE:HG12	1.93	0.49
1:K:5428:VAL:HG13	1:K:5544:VAL:HG22	1.94	0.49
1:A:1023:PRO:HB2	1:A:1034:LEU:HD21	1.95	0.49
1:A:1375:GLN:O	1:A:1378:ALA:HB3	2.12	0.49
1:A:1495:MET:HE1	1:A:1529:ILE:HG23	1.95	0.49
1:B:2359:ILE:HB	1:B:2360:PRO:HD3	1.91	0.49
1:C:3361:MET:SD	1:C:3361:MET:C	2.96	0.49
1:C:3540:LYS:O	1:C:3544:VAL:HG23	2.13	0.49
1:D:4024:PRO:HD3	1:D:4037:PHE:CD1	2.48	0.49
1:F:6375:GLN:HG3	1:F:6400:THR:HG22	1.94	0.49
1:G:1149:ALA:HB2	1:G:1168:ILE:O	2.12	0.49
1:G:1374:ASP:O	1:G:1376:LYS:N	2.46	0.49
1:H:2349:GLY:HA3	1:H:2447:TYR:CE1	2.48	0.49
1:H:2404:LEU:HD13	1:H:2413:LYS:CG	2.43	0.49
1:I:3330:LYS:NZ	1:I:3330:LYS:HB3	2.27	0.49
1:I:3355:PHE:CD1	1:I:3360:PRO:HG3	2.48	0.49
1:A:1304:LEU:HG	3:A:1:N LX:H151	1.93	0.49
1:B:2086:MET:HE3	1:B:2112:LEU:CD2	2.42	0.49
1:B:2452:ARG:NH1	4:B:7528:HOH:O	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:5068:PRO:HB3	1:E:5193:ASP:OD1	2.13	0.49
1:E:5404:LEU:HD22	1:E:5416:LEU:HB2	1.93	0.49
1:F:6478:ALA:N	1:F:6479:PRO:CD	2.75	0.49
1:G:1079:ASN:ND2	2:G:179:NAG:C1	2.76	0.49
1:G:1180:THR:HG22	1:G:1282:MET:HE2	1.94	0.49
1:H:2402:LYS:HG2	1:H:2546:PHE:CE1	2.47	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:K:5468:HIS:NE2	3:K:5:NLX:O3	2.46	0.49
1:L:6530:GLY:O	1:L:6531:ALA:C	2.56	0.49
1:B:2251:LEU:HB2	1:B:2429:PRO:HB3	1.95	0.49
1:D:4034:LEU:HD12	1:D:4079:ASN:OD1	2.13	0.49
1:G:1216:THR:OG1	1:G:1504:ALA:HA	2.12	0.49
1:G:1292:GLU:HG2	4:G:7529:HOH:O	2.11	0.49
1:G:1523:LYS:HB3	1:G:1537:GLN:OE1	2.12	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: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:L:6051:LEU:HD13	1:L:6083:TYR:CD1	2.48	0.49
1:L:6264:LEU:O	1:L:6268:ILE:HD13	2.12	0.49
1:A:1330:LYS:HB2	1:A:1335:LEU:CD2	2.43	0.48
1:C:3024:PRO:HG3	1:C:3037:PHE:CE1	2.47	0.48
1:C:3156:ALA:O	1:C:3160:HIS:HB2	2.13	0.48
1:C:3464:VAL:HG22	1:D:4370:GLU:OE1	2.13	0.48
1:E:5024:PRO:HD3	1:E:5037:PHE:CD1	2.47	0.48
1:E:5339:ARG:NH1	1:E:5339:ARG:HG2	2.28	0.48
1:G:1104:ARG:HH12	1:G:1153:ASP:HB2	1.78	0.48
1:G:1338:GLU:O	1:G:1340:ASN:N	2.46	0.48
1:H:2361:MET:HE3	1:H:2363:LEU:HG	1.95	0.48
1:J:4278:THR:OG1	1:J:4281:VAL:HG23	2.13	0.48
1:K:5361:MET:SD	1:K:5363:LEU:HG	2.52	0.48
1:L:6304:LEU:HB3	3:L:6:NLX:H172	1.94	0.48
1:B:2079:ASN:HD21	2:B:279:NAG:C1	2.26	0.48
1:B:2308:LEU:HD22	1:E:5459:MET:SD	2.53	0.48
1:B:2370:GLU:O	1:B:2372:GLN:HG3	2.13	0.48
1:B:2549:ASN:O	1:B:2550:LEU:C	2.56	0.48
1:D:4309:GLN:NE2	1:D:4310:GLY:N	2.61	0.48
1:E:5452:ARG:HE	1:E:5462:LYS:HA	1.78	0.48
1:K:5359:ILE:HG12	3:K:5:NLX:H151	1.96	0.48
1:A:1405:GLY:O	1:A:1406:GLY:C	2.56	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2254:VAL:HG21	1:B:2388:LEU:HD23	1.95	0.48
1:C:3257:LYS:HE3	1:C:3322:VAL:HG12	1.95	0.48
1:E:5176:GLY:HA2	1:E:5189:TRP:HB2	1.95	0.48
1:E:5538:LYS:HB3	1:E:5541:ASP:HB2	1.95	0.48
1:F:6202:GLN:NE2	1:F:6212:PRO:O	2.46	0.48
1:G:1142:GLY:CA	3:G:1:NLX:H152	2.43	0.48
1:H:2237:LYS:O	1:H:2238:ASN:HB2	2.11	0.48
1:J:4187:GLY:O	1:J:4188:ASN:HB2	2.13	0.48
1:K:5215:VAL:H	1:K:5241:HIS:CD2	2.19	0.48
1:K:5380:SER:O	1:K:5384:LYS:HG2	2.13	0.48
1:K:5420:LEU:CD1	1:K:5547:TRP:HZ2	2.24	0.48
1:A:1068:PRO:HA	4:A:7198:HOH:O	2.13	0.48
1:A:1304:LEU:HG	3:A:1:NLX:O4	2.12	0.48
1:E:5361:MET:C	1:E:5361:MET:SD	2.97	0.48
1:L:6478:ALA:N	1:L:6479:PRO:CD	2.76	0.48
1:A:1358:LEU:O	1:A:1363:LEU:HD12	2.14	0.48
1:B:2255:LEU:HD23	1:B:2318:LEU:HD13	1.94	0.48
1:B:2491:ARG:O	1:B:2492:LEU:C	2.55	0.48
1:C:3112:LEU:O	1:C:3113:SER:HB2	2.13	0.48
1:D:4551:PHE:C	1:D:4553:LYS:H	2.22	0.48
1:F:6512:GLU:CD	1:F:6512:GLU:N	2.71	0.48
1:G:1318:LEU:HD12	1:G:1318:LEU:O	2.12	0.48
1:I:3251:LEU:HD21	1:I:3333:GLU:HG3	1.96	0.48
1:I:3251:LEU:HD12	1:I:3433:VAL:CG2	2.44	0.48
1:I:3391:ILE:O	1:I:3392:ALA:C	2.57	0.48
1:K:5225:GLU:C	1:K:5225:GLU:OE1	2.56	0.48
1:K:5353:GLN:O	1:K:5467:ASP:HA	2.13	0.48
1:K:5478:ALA:N	1:K:5479:PRO:CD	2.76	0.48
1:A:1251:LEU:HD12	1:A:1433:VAL:CG2	2.43	0.48
1:A:1311:ASP:OD1	1:A:1313:ARG:HB2	2.14	0.48
1:B:2520:TYR:CZ	1:B:2524:GLU:HG2	2.49	0.48
1:C:3290:THR:HG23	1:C:3293:GLU:OE2	2.12	0.48
1:F:6136:MET:HB3	1:F:6218:PHE:HE1	1.79	0.48
1:F:6188:ASN:ND2	1:F:6324:ASP:OD2	2.44	0.48
1:G:1304:LEU:CG	3:G:1:NLX:H203	2.36	0.48
1:G:1308:LEU:HD22	1:L:6459:MET:SD	2.53	0.48
1:H:2027:ASP:CG	1:H:2032:LYS:HZ1	2.22	0.48
1:H:2297:THR:O	1:H:2301:MET:HG2	2.14	0.48
1:J:4145:MET:HG3	1:J:4304:LEU:HD11	1.96	0.48
1:K:5349:GLY:HA3	1:K:5447:TYR:CE1	2.49	0.48
1:K:5370:GLU:C	1:K:5372:GLN:N	2.72	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2292:GLU:O	1:B:2296:GLU:HG3	2.13	0.48
1:D:4420:LEU:C	1:D:4420:LEU:CD1	2.87	0.48
1:E:5286:LEU:HA	1:E:5289:LYS:HG3	1.96	0.48
1:G:1140:HIS:CD2	1:G:1147:GLY:HA3	2.48	0.48
1:H:2101:PHE:CE2	3:H:2:N LX:H21	2.49	0.48
1:L:6182:ASP:HB2	1:L:6183:GLU:OE2	2.14	0.48
1:A:1024:PRO:HD3	1:A:1037:PHE:CD1	2.48	0.48
1:A:1268:ILE:HG12	1:A:1301:MET:HE2	1.96	0.48
1:A:1284:HIS:O	1:A:1288:GLN:OE1	2.32	0.48
1:B:2143:GLY:O	1:B:2144:LEU:HB2	2.14	0.48
1:C:3026:VAL:HG13	4:C:7260:HOH:O	2.13	0.48
1:D:4140:HIS:HD2	1:D:4141:GLY:O	1.97	0.48
1:E:5086:MET:HE2	1:E:5112:LEU:CD2	2.44	0.48
1:E:5338:GLU:HG3	1:E:5338:GLU:O	2.13	0.48
1:F:6086:MET:HE3	1:F:6112:LEU:HD21	1.96	0.48
1:K:5099:GLU:HG3	1:K:5107:ASN:OD1	2.13	0.48
1:K:5217:ILE:O	1:K:5243:ALA:HA	2.14	0.48
1:L:6324:ASP:OD1	1:L:6327:LEU:N	2.36	0.48
1:L:6492:LEU:O	1:L:6496:VAL:HG23	2.14	0.48
1:B:2174:ILE:CG1	1:B:2298:THR:HG22	2.44	0.48
1:B:2318:LEU:CD1	3:B:2:N LX:H171	2.43	0.48
1:B:2499:PHE:HZ	1:B:2515:PRO:HG2	1.78	0.48
1:C:3475:VAL:HG22	1:C:3496:VAL:HG11	1.96	0.48
1:D:4143:GLY:O	1:D:4145:MET:HG2	2.13	0.48
1:E:5215:VAL:H	1:E:5241:HIS:CD2	2.28	0.48
1:E:5465:ILE:HD12	1:E:5465:ILE:N	2.29	0.48
1:E:5502:ASN:O	1:E:5506:ASN:HB2	2.14	0.48
1:F:6107:ASN:HD22	1:F:6108:ILE:H	1.62	0.48
1:F:6359:ILE:HG12	3:F:6:N LX:C15	2.43	0.48
1:G:1374:ASP:O	1:G:1375:GLN:C	2.56	0.48
1:H:2143:GLY:HA3	3:H:2:N LX:C15	2.44	0.48
1:H:2363:LEU:HD22	3:H:2:N LX:H181	1.94	0.48
1:H:2478:ALA:N	1:H:2479:PRO:CD	2.77	0.48
1:I:3324:ASP:OD2	1:I:3327:LEU:HB3	2.13	0.48
1:I:3350:ILE:C	1:I:3351:ASN:HD22	2.22	0.48
1:J:4079:ASN:ND2	2:J:479:NAG:H5	2.26	0.48
1:K:5087:CYS:O	1:K:5088:THR:C	2.57	0.48
1:K:5104:ARG:HG2	1:K:5104:ARG:HH11	1.78	0.48
1:K:5404:LEU:O	1:K:5413:LYS:HE2	2.13	0.48
1:A:1040:LEU:HD22	1:A:1156:ALA:HA	1.96	0.48
1:B:2447:TYR:CD2	1:B:2447:TYR:C	2.91	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2453:PRO:C	1:B:2455:PHE:H	2.22	0.48
1:C:3436:ASN:N	1:C:3436:ASN:ND2	2.61	0.48
1:C:3543:GLU:OE2	1:C:3543:GLU:N	2.42	0.48
1:D:4461:PRO:HG2	1:D:4464:VAL:CG2	2.44	0.48
1:E:5039:SER:OG	1:E:5046:PRO:HG3	2.14	0.48
1:E:5187:GLY:O	1:E:5188:ASN:HB2	2.14	0.48
1:E:5404:LEU:HD22	1:E:5413:LYS:O	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:H:2311:ASP:HB3	1:H:2314:GLU:HG2	1.96	0.48
1:I:3352:LYS:HE3	1:I:3450:GLN:CD	2.38	0.48
1:J:4130:LYS:HD3	1:J:4131:ASN:N	2.27	0.48
1:J:4353:GLN:NE2	1:J:4465:ILE:H	2.12	0.48
1:K:5309:GLN:NE2	4:K:7219:HOH:O	2.42	0.48
1:A:1024:PRO:HB3	1:A:1037:PHE:CZ	2.49	0.47
1:A:1128:THR:HG23	4:A:7990:HOH:O	2.13	0.47
1:B:2223:GLY:O	1:B:2227:VAL:HG23	2.14	0.47
1:D:4296:GLU:O	1:D:4300:LYS:HG3	2.14	0.47
1:D:4382:LEU:HD11	1:D:4391:ILE:HD12	1.95	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:G:1104:ARG:CZ	1:G:1153:ASP:HB2	2.43	0.47
1:G:1161:GLU:OE2	1:G:1498:LYS:HG2	2.14	0.47
1:H:2143:GLY:O	1:H:2318:LEU:HD22	2.14	0.47
1:H:2338:GLU:HB3	1:H:2340:ASN:OD1	2.14	0.47
1:I:3492:LEU:O	1:I:3496:VAL:HG23	2.14	0.47
1:K:5100:LEU:HD22	1:K:5457:SER:HB2	1.96	0.47
1:G:1134:PRO:CG	1:G:1163:VAL:HG12	2.29	0.47
1:H:2225:GLU:O	1:H:2228:SER:N	2.47	0.47
1:H:2368:LEU:HB2	1:K:5369:SER:HA	1.95	0.47
1:H:2385:SER:O	1:H:2389:VAL:HG22	2.15	0.47
1:I:3237:LYS:O	1:I:3238:ASN:HB2	2.14	0.47
1:J:4319:LEU:N	1:J:4319:LEU:HD23	2.28	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:F:6409:ASP:OD2	1:F:6412:LYS:HB2	2.14	0.47
1:G:1034:LEU:O	1:G:1081:THR:HG23	2.15	0.47
1:I:3044:ALA:O	1:I:3046:PRO:HD3	2.13	0.47
1:J:4218:PHE:N	1:J:4218:PHE:CD1	2.82	0.47
1:J:4349:GLY:HA3	1:J:4447:TYR:CE1	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:4412:LYS:O	1:J:4416:LEU:HG	2.14	0.47
1:J:4417:PHE:O	1:J:4420:LEU:HB3	2.14	0.47
1:A:1249:VAL:HB	1:A:1433:VAL:HG21	1.96	0.47
1:B:2220:GLU:OE1	1:B:2221:SER:CB	2.58	0.47
1:C:3092:LYS:HD2	1:D:4302:LYS:HD2	1.97	0.47
1:C:3304:LEU:HD22	3:C:3:NLX:C20	2.43	0.47
1:E:5257:LYS:HA	4:E:7588:HOH:O	2.13	0.47
1:F:6396:ILE:HB	1:F:6397:PRO:HD3	1.96	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:J:4363:LEU:CD1	3:J:4:NLX:H181	2.32	0.47
1:L:6533:THR:C	1:L:6534:GLN:HG3	2.39	0.47
1:A:1119:LEU:HD12	1:A:1119:LEU:O	2.15	0.47
1:A:1309:GLN:HE21	1:A:1309:GLN:C	2.22	0.47
1:F:6107:ASN:ND2	1:F:6108:ILE:N	2.62	0.47
1:F:6375:GLN:HG3	1:F:6400:THR:CG2	2.45	0.47
1:G:1349:GLY:HA3	1:G:1447:TYR:CZ	2.50	0.47
1:G:1547:TRP:CZ3	1:G:1550:LEU:HD23	2.50	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:I:3318:LEU:HG	3:I:3:NLX:C18	2.44	0.47
1:I:3364:MET:CG	3:I:3:NLX:H201	2.43	0.47
1:J:4183:GLU:OE2	1:J:4183:GLU:N	2.47	0.47
1:K:5104:ARG:NH1	1:K:5104:ARG:HG2	2.29	0.47
1:K:5354:GLU:HB2	1:K:5422:ALA:HB1	1.96	0.47
1:L:6414:LYS:O	1:L:6418:LEU:HG	2.14	0.47
1:A:1218:PHE:HB3	1:A:1244:ILE:HB	1.94	0.47
1:A:1375:GLN:NE2	1:A:1400:THR:HG22	2.25	0.47
1:C:3034:LEU:C	1:C:3034:LEU:HD13	2.40	0.47
1:C:3402:LYS:HG2	1:C:3546:PHE:CE1	2.49	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:I:3258:LYS:H	1:I:3258:LYS:CE	2.27	0.47
1:J:4119:LEU:HD12	1:J:4119:LEU:C	2.39	0.47
1:J:4277:THR:HG21	1:L:6113:SER:HB2	1.96	0.47
1:J:4302:LYS:HB3	1:J:4302:LYS:HZ3	1.77	0.47
1:J:4449:PHE:CE2	1:J:4471:GLU:HA	2.50	0.47
1:K:5363:LEU:HD13	3:K:5:NLX:C20	2.45	0.47
1:K:5549:ASN:O	1:K:5552:ALA:HB3	2.15	0.47
1:L:6145:MET:HE1	1:L:6303:PHE:CD1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:6447:TYR:HB3	1:L:6517:TRP:CZ2	2.50	0.47
1:A:1201:VAL:O	1:A:1205:ILE:HB	2.14	0.47
1:A:1296:GLU:O	1:A:1300:LYS:HG3	2.15	0.47
1:B:2092:LYS:HD2	1:E:5302:LYS:HE3	1.97	0.47
1:D:4145:MET:CG	1:D:4304:LEU:HD11	2.45	0.47
1:D:4188:ASN:HD22	1:D:4324:ASP:CG	2.22	0.47
1:D:4478:ALA:HB3	1:D:4479:PRO:HD3	1.96	0.47
1:E:5339:ARG:HG2	1:E:5339:ARG:HH11	1.80	0.47
1:E:5363:LEU:HB3	3:E:5:N LX:C20	2.35	0.47
1:E:5456:SER:HB3	1:E:5460:LYS:HD2	1.97	0.47
1:G:1241:HIS:O	1:G:1242:ARG:HD3	2.15	0.47
1:G:1380:SER:O	1:G:1383:TRP:HB3	2.15	0.47
1:H:2366:TYR:OH	1:H:2385:SER:HB3	2.15	0.47
1:H:2417:PHE:O	1:H:2420:LEU:HB3	2.15	0.47
1:I:3191:HIS:CD2	1:I:3321:THR:HG23	2.50	0.47
1:I:3301:MET:HB2	1:I:3303:PHE:CE1	2.49	0.47
1:I:3366:TYR:HA	1:I:3367:PRO:HD3	1.76	0.47
1:J:4258:LYS:HD3	1:J:4258:LYS:N	2.30	0.47
1:J:4264:LEU:HG	1:J:4316:GLN:HG2	1.96	0.47
1:J:4312:PRO:C	1:J:4314:GLU:H	2.23	0.47
1:J:4398:GLU:OE2	1:J:4550:LEU:HD13	2.15	0.47
1:L:6145:MET:HB3	1:L:6304:LEU:HD11	1.96	0.47
1:L:6290:THR:O	1:L:6291:GLU:C	2.58	0.47
1:L:6363:LEU:HD22	3:L:6:N LX:C20	2.44	0.47
1:L:6526:TYR:CZ	1:L:6536:ALA:HB3	2.50	0.47
1:A:1304:LEU:HD12	1:A:1318:LEU:HD23	1.96	0.47
1:B:2366:TYR:HD2	1:B:2368:LEU:HD13	1.79	0.47
1:B:2367:PRO:C	1:B:2368:LEU:HD12	2.40	0.47
1:G:1262:LYS:HB3	1:G:1263:PRO:HD3	1.97	0.47
1:G:1508:ASN:OD1	1:G:1510:ASN:HB2	2.15	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: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:D:4143:GLY:C	1:D:4145:MET:H	2.23	0.47
1:G:1140:HIS:HE1	4:G:7298:HOH:O	1.97	0.47
1:G:1302:LYS:CG	1:L:6092:LYS:HZ3	2.20	0.47
1:G:1354:GLU:HG3	1:G:1426:PHE:HB2	1.97	0.47
1:H:2101:PHE:HE2	3:H:2:N LX:H21	1.80	0.47
1:H:2126:ASP:OD1	1:H:2128:THR:HG23	2.14	0.47
1:I:3024:PRO:HG3	1:I:3037:PHE:CZ	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:3125:ALA:HB2	1:I:3133:LEU:CD1	2.45	0.47
1:I:3221:SER:OG	1:I:3222:ALA:N	2.47	0.47
1:I:3381:LEU:CD2	1:J:4459:MET:HG2	2.44	0.47
1:I:3420:LEU:C	1:I:3420:LEU:HD12	2.40	0.47
1:J:4218:PHE:N	1:J:4218:PHE:HD1	2.12	0.47
1:K:5254:VAL:O	1:K:5254:VAL:HG22	2.15	0.47
1:K:5264:LEU:HD22	1:K:5316:GLN:NE2	2.29	0.47
1:L:6339:ARG:HH21	1:L:6439:ASP:HB2	1.80	0.47
1:A:1304:LEU:CD2	3:A:1:NLX:H151	2.45	0.47
1:E:5083:TYR:CE2	1:E:5108:ILE:HD13	2.49	0.47
1:E:5114:GLU:HG3	1:E:5291:GLU:OE2	2.16	0.47
1:G:1087:CYS:HB3	4:G:7585:HOH:O	2.15	0.47
1:G:1201:VAL:O	1:G:1205:ILE:HB	2.14	0.47
1:H:2179:SER:O	1:H:2265:ALA:HB2	2.15	0.47
1:H:2363:LEU:CB	3:H:2:NLX:H181	2.25	0.47
1:K:5089:GLN:O	1:K:5090:ASP:C	2.57	0.47
1:L:6029:VAL:HG13	4:L:7981:HOH:O	2.15	0.47
1:D:4304:LEU:HB3	3:D:4:NLX:C20	2.40	0.46
1:E:5437:HIS:CD2	1:E:5444:THR:OG1	2.69	0.46
1:G:1513:GLY:O	1:G:1514:LEU:HD23	2.15	0.46
1:H:2375:GLN:NE2	1:H:2400:THR:HG22	2.30	0.46
1:J:4107:ASN:HD22	1:J:4108:ILE:N	2.12	0.46
1:K:5068:PRO:HB3	1:K:5193:ASP:OD1	2.14	0.46
1:K:5258:LYS:N	1:K:5258:LYS:CD	2.71	0.46
1:K:5407:THR:OG1	1:K:5408:ASP:N	2.48	0.46
1:L:6136:MET:HB3	1:L:6218:PHE:CE1	2.50	0.46
1:L:6435:ARG:NH1	1:L:6544:VAL:HG11	2.30	0.46
1:L:6480:PHE:N	1:L:6480:PHE:CD1	2.83	0.46
1:L:6499:PHE:HD2	1:L:6509:PRO:O	1.99	0.46
3:B:2:NLX:H203	3:B:2:NLX:O4	2.15	0.46
1:D:4041:GLU:HB3	4:D:7218:HOH:O	2.14	0.46
1:E:5183:GLU:OE2	1:E:5183:GLU:N	2.41	0.46
1:F:6143:GLY:O	1:F:6145:MET:HG2	2.15	0.46
1:G:1543:GLU:O	1:G:1547:TRP:CD1	2.68	0.46
1:I:3426:PHE:HE2	3:I:3:NLX:HO11	1.62	0.46
1:J:4086:MET:HE3	1:J:4112:LEU:HD21	1.96	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:E:5540:LYS:O	1:E:5544:VAL:HG23	2.15	0.46
1:I:3338:GLU:C	1:I:3340:ASN:N	2.71	0.46
1:K:5395:LEU:HD13	1:K:5550:LEU:HD23	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2403:TYR:O	1:B:2416:LEU:HD13	2.15	0.46
1:B:2495:MET:HE3	1:B:2499:PHE:CE1	2.51	0.46
1:C:3427:GLY:O	1:C:3428:VAL:C	2.59	0.46
1:F:6330:LYS:HG3	1:F:6335:LEU:CD2	2.44	0.46
1:G:1437:HIS:O	1:G:1440:ALA:HB3	2.16	0.46
1:G:1438:ARG:NH1	1:G:1524:GLU:HG2	2.31	0.46
1:H:2359:ILE:HG12	3:H:2:NLX:C8	2.46	0.46
1:I:3368:LEU:O	1:J:4369:SER:HA	2.14	0.46
1:J:4274:CYS:SG	1:J:4285:CYS:SG	3.04	0.46
1:J:4318:LEU:HD12	1:J:4318:LEU:O	2.16	0.46
1:K:5550:LEU:C	1:K:5552:ALA:N	2.74	0.46
1:L:6416:LEU:O	1:L:6419:ASP:HB2	2.15	0.46
1:A:1129:LYS:HD3	4:A:7882:HOH:O	2.15	0.46
1:D:4079:ASN:CG	2:D:479:NAG:C1	2.88	0.46
1:F:6120:ASN:HB2	1:F:6167:THR:OG1	2.16	0.46
1:G:1211:ASN:HD22	1:G:1214:SER:HB3	1.80	0.46
1:H:2386:TYR:N	1:H:2387:PRO:CD	2.78	0.46
1:I:3218:PHE:CD1	1:I:3218:PHE:N	2.84	0.46
1:K:5183:GLU:OE2	1:K:5183:GLU:N	2.44	0.46
1:K:5264:LEU:HD22	1:K:5316:GLN:HE21	1.80	0.46
1:K:5401:GLU:O	1:K:5402:LYS:C	2.58	0.46
1:K:5447:TYR:HB3	1:K:5517:TRP:CZ2	2.51	0.46
1:L:6107:ASN:HD22	1:L:6108:ILE:N	2.13	0.46
1:L:6363:LEU:HB3	3:L:6:NLX:C20	2.44	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:A:1394:GLU:O	1:A:1397:PRO:HD2	2.14	0.46
1:B:2452:ARG:HG2	1:B:2452:ARG:NH1	2.29	0.46
1:D:4040:LEU:O	1:D:4041:GLU:C	2.57	0.46
1:E:5343:THR:HB	1:E:5442:ALA:HB2	1.98	0.46
1:G:1216:THR:HG23	1:G:1242:ARG:HB2	1.96	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:J:4492:LEU:HD12	1:J:4495:MET:HE2	1.98	0.46
1:K:5160:HIS:CE1	1:K:5480:PHE:CE2	3.04	0.46
1:A:1267:GLN:OE1	1:A:1301:MET:HE1	2.16	0.46
1:B:2218:PHE:HB3	1:B:2244:ILE:HB	1.98	0.46
1:B:2428:VAL:HG13	1:B:2544:VAL:HG22	1.96	0.46
1:C:3375:GLN:HE21	1:C:3375:GLN:HB3	1.57	0.46
1:C:3534:GLN:N	1:C:3534:GLN:CD	2.73	0.46
1:E:5373:LEU:H	1:E:5410:THR:HB	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:5491:ARG:NE	4:E:7007:HOH:O	2.42	0.46
1:A:1152:TYR:N	1:A:1152:TYR:CD1	2.84	0.46
1:B:2258:LYS:O	1:B:2258:LYS:HD2	2.16	0.46
1:B:2304:LEU:HD23	3:B:2:NLX:H191	1.98	0.46
1:C:3140:HIS:HD2	1:C:3141:GLY:O	1.97	0.46
1:E:5358:LEU:HG	1:E:5363:LEU:HD12	1.98	0.46
1:F:6359:ILE:CD1	3:F:6:NLX:H151	2.45	0.46
1:G:1119:LEU:C	1:G:1119:LEU:HD12	2.41	0.46
1:G:1536:ALA:O	1:G:1537:GLN:HG2	2.16	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:I:3096:LEU:HD13	1:J:4309:GLN:HB2	1.98	0.46
1:J:4375:GLN:HE21	1:J:4375:GLN:HB3	1.55	0.46
1:L:6060:LEU:CD2	1:L:6114:GLU:HB3	2.45	0.46
1:A:1220:GLU:HA	1:A:1246:GLU:O	2.16	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:B:2458:ASP:HB2	4:E:7333:HOH:O	2.16	0.46
1:C:3445:TYR:CZ	1:C:3509:PRO:HD2	2.51	0.46
1:C:3501:ALA:O	1:C:3505:ARG:HG2	2.14	0.46
1:E:5242:ARG:HG3	1:E:5242:ARG:NH1	2.28	0.46
1:F:6103:ASN:ND2	1:F:6476:PHE:HB3	2.31	0.46
1:F:6262:LYS:NZ	1:F:6282:MET:HE1	2.30	0.46
1:F:6296:GLU:O	1:F:6300:LYS:HG3	2.15	0.46
1:F:6349:GLY:HA3	1:F:6447:TYR:CE1	2.51	0.46
1:G:1145:MET:HG3	1:G:1304:LEU:HD21	1.98	0.46
1:G:1352:LYS:HD3	1:G:1450:GLN:CD	2.41	0.46
1:G:1355:PHE:CD1	1:G:1360:PRO:HG3	2.50	0.46
1:I:3103:ASN:HD22	1:I:3481:LEU:HD12	1.80	0.46
1:L:6161:GLU:HB3	1:L:6501:ALA:CB	2.46	0.46
1:L:6205:ILE:HA	1:L:6205:ILE:HD12	1.69	0.46
1:L:6452:ARG:HG2	1:L:6452:ARG:HH11	1.81	0.46
1:A:1104:ARG:NH1	1:A:1153:ASP:HB2	2.29	0.46
1:A:1334:GLU:O	1:A:1337:ALA:HB3	2.16	0.46
1:C:3407:THR:HG21	1:C:3412:LYS:HZ3	1.79	0.46
1:D:4251:LEU:HD12	1:D:4433:VAL:HG23	1.96	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:2087:CYS:HB3	4:H:7192:HOH:O	2.15	0.46
1:J:4256:VAL:HG12	1:J:4258:LYS:HD2	1.98	0.46
1:K:5428:VAL:N	1:K:5429:PRO:CD	2.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:2417:PHE:O	1:B:2420:LEU:HB3	2.15	0.45
1:E:5354:GLU:O	1:E:5468:HIS:HB2	2.17	0.45
1:E:5492:LEU:HD12	1:E:5495:MET:HE2	1.99	0.45
1:G:1103:ASN:ND2	1:G:1476:PHE:HB3	2.31	0.45
1:H:2143:GLY:O	1:H:2144:LEU:HB2	2.16	0.45
1:H:2346:TYR:HD2	1:H:2347:MET:N	2.14	0.45
1:I:3161:GLU:HB3	1:I:3501:ALA:CB	2.46	0.45
1:J:4143:GLY:N	3:J:4:NLX:H152	2.31	0.45
1:J:4447:TYR:C	1:J:4447:TYR:CD2	2.94	0.45
1:K:5212:PRO:HG2	4:K:7443:HOH:O	2.16	0.45
1:K:5395:LEU:HD23	4:K:7575:HOH:O	2.15	0.45
1:L:6187:GLY:O	1:L:6188:ASN:HB2	2.16	0.45
1:L:6304:LEU:HD13	3:L:6:NLX:C19	2.46	0.45
1:L:6351:ASN:ND2	4:L:7041:HOH:O	2.49	0.45
1:B:2124:PRO:HD3	1:B:2158:ALA:HB1	1.98	0.45
1:B:2540:LYS:O	1:B:2544:VAL:HG23	2.16	0.45
1:C:3355:PHE:CE1	1:C:3421:ILE:HG21	2.50	0.45
1:C:3409:ASP:HB3	1:C:3412:LYS:HB3	1.98	0.45
1:E:5091:PRO:HG3	1:E:5112:LEU:CD1	2.37	0.45
1:F:6338:GLU:C	1:F:6340:ASN:N	2.72	0.45
1:H:2190:GLY:O	1:H:2193:ASP:HB2	2.16	0.45
1:I:3123:THR:OG1	1:I:3164:VAL:HG22	2.16	0.45
1:J:4420:LEU:HD12	1:J:4547:TRP:HZ2	1.81	0.45
1:K:5318:LEU:HD11	3:K:5:NLX:H21	1.98	0.45
1:K:5431:VAL:O	1:K:5435:ARG:HG3	2.16	0.45
1:L:6244:ILE:HG12	1:L:6347:MET:HB3	1.98	0.45
1:L:6349:GLY:HA3	1:L:6447:TYR:CZ	2.52	0.45
1:A:1289:LYS:HD3	4:A:8105:HOH:O	2.16	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:D:4182:ASP:HB2	1:D:4183:GLU:OE2	2.16	0.45
1:D:4215:VAL:N	1:D:4241:HIS:HD2	1.97	0.45
1:E:5086:MET:HE3	1:E:5089:GLN:NE2	2.31	0.45
1:H:2338:GLU:O	1:H:2339:ARG:HD3	2.17	0.45
1:H:2409:ASP:C	1:H:2411:VAL:H	2.25	0.45
1:I:3217:ILE:HD12	1:I:3227:VAL:HG13	1.99	0.45
1:I:3383:TRP:CZ3	1:I:3393:LYS:HB2	2.51	0.45
1:J:4073:PRO:HB2	4:J:7805:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:4251:LEU:HD12	1:J:4433:VAL:CG2	2.46	0.45
1:J:4498:LYS:HB3	1:J:4514:LEU:HD11	1.98	0.45
1:K:5368:LEU:HD12	1:K:5368:LEU:N	2.31	0.45
1:K:5404:LEU:C	1:K:5406:GLY:H	2.23	0.45
1:K:5409:ASP:OD2	1:K:5412:LYS:HG3	2.16	0.45
1:B:2218:PHE:HB2	1:B:2244:ILE:HB	1.99	0.45
1:G:1179:SER:O	1:G:1265:ALA:HB2	2.16	0.45
1:I:3104:ARG:CZ	1:I:3153:ASP:HB2	2.46	0.45
1:J:4455:PHE:CD2	1:J:4482:LYS:HD3	2.50	0.45
1:A:1179:SER:OG	1:A:1186:ARG:O	2.32	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:3092:LYS:NZ	1:D:4302:LYS:HD2	2.32	0.45
1:C:3220:GLU:HA	1:C:3246:GLU:O	2.16	0.45
1:E:5051:LEU:O	1:E:5080:ALA:HB1	2.16	0.45
1:E:5252:THR:HG22	1:E:5254:VAL:HG12	1.98	0.45
1:F:6366:TYR:HA	1:F:6367:PRO:HD3	1.81	0.45
1:I:3087:CYS:O	1:I:3088:THR:C	2.59	0.45
1:I:3492:LEU:HD12	1:I:3495:MET:HE2	1.99	0.45
1:K:5100:LEU:CD2	1:K:5457:SER:HB2	2.47	0.45
1:K:5414:LYS:HE2	1:K:5414:LYS:HB3	1.80	0.45
1:K:5486:SER:O	1:K:5490:ILE:HG13	2.17	0.45
1:L:6149:ALA:CB	1:L:6169:GLN:HG3	2.47	0.45
1:B:2372:GLN:NE2	1:E:5463:THR:HG21	2.32	0.45
1:D:4038:VAL:CG2	1:D:4049:ILE:HD12	2.45	0.45
1:D:4234:PRO:O	1:D:4237:LYS:HB2	2.17	0.45
1:E:5174:ILE:HA	1:E:5319:LEU:HD13	1.99	0.45
1:I:3266:GLU:O	1:I:3270:ILE:HG13	2.17	0.45
1:J:4023:PRO:CB	1:J:4034:LEU:HD21	2.46	0.45
1:J:4089:GLN:OE1	1:J:4146:VAL:HB	2.17	0.45
1:J:4093:ALA:HB1	3:J:4:NLX:H191	1.98	0.45
1:J:4370:GLU:C	1:J:4372:GLN:H	2.24	0.45
1:K:5237:LYS:HA	1:K:5237:LYS:CE	2.31	0.45
1:K:5386:TYR:N	1:K:5387:PRO:HD2	2.32	0.45
1:L:6348:VAL:O	1:L:6446:MET:HA	2.17	0.45
1:L:6545:ALA:C	1:L:6548:THR:HG22	2.42	0.45
1:A:1370:GLU:OE2	1:A:1370:GLU:HA	2.16	0.45
1:B:2260:ASP:OD1	1:B:2263:PRO:HD3	2.16	0.45
1:B:2389:VAL:HB	1:B:2424:VAL:HG11	1.98	0.45
1:C:3107:ASN:ND2	1:C:3108:ILE:H	2.14	0.45
1:C:3357:TRP:C	1:C:3360:PRO:HD2	2.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3361:MET:CE	1:C:3363:LEU:HG	2.47	0.45
1:D:4049:ILE:HD11	1:D:4155:LEU:HD13	1.98	0.45
1:D:4186:ARG:HH11	1:D:4186:ARG:HG3	1.82	0.45
1:D:4221:SER:CB	3:D:4:NLX:O1	2.65	0.45
1:E:5087:CYS:O	1:E:5088:THR:C	2.58	0.45
1:F:6218:PHE:HB3	1:F:6244:ILE:HB	1.99	0.45
1:F:6534:GLN:CD	1:F:6534:GLN:H	2.24	0.45
1:G:1180:THR:HB	1:G:1279:SER:OG	2.17	0.45
1:G:1304:LEU:HD12	1:G:1318:LEU:HD23	1.96	0.45
1:G:1351:ASN:O	1:G:1352:LYS:C	2.60	0.45
1:G:1395:LEU:HD22	1:G:1550:LEU:CD1	2.47	0.45
1:H:2187:GLY:O	1:H:2188:ASN:HB2	2.17	0.45
1:H:2423:ASP:O	1:H:2428:VAL:HG23	2.15	0.45
1:H:2528:GLN:HB2	1:H:2534:GLN:HE21	1.82	0.45
1:I:3143:GLY:HA2	1:I:3222:ALA:HB2	1.99	0.45
1:I:3201:VAL:HB	4:I:7603:HOH:O	2.16	0.45
1:J:4304:LEU:CB	3:J:4:NLX:H203	2.46	0.45
1:K:5091:PRO:HG3	1:K:5112:LEU:CD2	2.46	0.45
1:L:6156:ALA:HB3	4:L:8057:HOH:O	2.17	0.45
1:L:6500:TRP:N	1:L:6500:TRP:HE3	2.15	0.45
1:D:4105:LYS:HG3	1:D:4481:LEU:O	2.16	0.45
1:F:6130:LYS:NZ	4:F:7489:HOH:O	2.38	0.45
1:G:1524:GLU:O	1:G:1538:LYS:N	2.50	0.45
1:H:2143:GLY:CA	3:H:2:NLX:H152	2.46	0.45
1:H:2311:ASP:HA	1:H:2312:PRO:HD3	1.80	0.45
1:K:5026:VAL:CG1	1:K:5027:ASP:N	2.80	0.45
1:K:5526:TYR:CE2	1:K:5536:ALA:HB3	2.52	0.45
1:L:6121:ILE:HG22	1:L:6122:TYR:N	2.32	0.45
1:L:6501:ALA:O	1:L:6504:ALA:HB3	2.17	0.45
1:A:1043:PHE:CD2	1:L:6484:GLY:HA2	2.52	0.45
1:C:3214:SER:HA	1:C:3241:HIS:CD2	2.52	0.45
1:E:5034:LEU:C	1:E:5034:LEU:CD2	2.90	0.45
1:E:5336:GLN:HE22	1:E:5433:VAL:HA	1.82	0.45
1:F:6049:ILE:HG12	1:F:6122:TYR:CD2	2.52	0.45
1:F:6086:MET:HE3	1:F:6112:LEU:CD2	2.47	0.45
1:F:6268:ILE:HD11	1:F:6319:LEU:HD21	1.97	0.45
1:F:6528:GLN:O	1:F:6533:THR:HG23	2.16	0.45
1:G:1338:GLU:O	1:G:1339:ARG:C	2.59	0.45
1:G:1373:LEU:HG	1:G:1378:ALA:HB2	1.98	0.45
1:G:1540:LYS:O	1:G:1544:VAL:HG23	2.17	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:J:4303:PHE:C	1:J:4304:LEU:HD22	2.41	0.45
1:K:5057:LYS:HG3	1:K:5058:PRO:CD	2.47	0.45
1:K:5125:ALA:HB1	1:K:5131:ASN:ND2	2.32	0.45
1:K:5240:PHE:N	1:K:5240:PHE:CD1	2.85	0.45
1:K:5385:SER:C	1:K:5387:PRO:HD2	2.42	0.45
1:L:6235:LEU:CD1	1:L:6327:LEU:HA	2.47	0.45
1:C:3220:GLU:HG2	1:C:3472:LEU:HD21	1.98	0.45
1:E:5403:TYR:O	1:E:5416:LEU:HD13	2.17	0.45
1:E:5407:THR:HG21	1:E:5412:LYS:CB	2.41	0.45
1:F:6283:VAL:O	1:F:6287:ARG:HG3	2.16	0.45
1:G:1079:ASN:CB	2:G:179:NAG:H82	2.34	0.45
1:G:1467:ASP:HB3	1:G:1470:ASP:OD1	2.17	0.45
1:I:3057:LYS:HD3	1:I:3063:LEU:CD1	2.46	0.45
1:I:3359:ILE:HB	1:I:3360:PRO:HD3	1.98	0.45
1:J:4361:MET:C	1:J:4361:MET:SD	3.00	0.45
1:K:5125:ALA:HB2	1:K:5133:LEU:HD12	1.98	0.45
1:K:5318:LEU:HD21	3:K:5:N LX:H11	1.97	0.45
1:K:5487:GLU:HG2	4:K:8070:HOH:O	2.17	0.45
1:L:6251:LEU:HD21	1:L:6333:GLU:HG3	1.98	0.45
1:L:6286:LEU:O	1:L:6289:LYS:HB2	2.16	0.45
1:L:6526:TYR:CE2	1:L:6539:LEU:HA	2.51	0.45
1:A:1375:GLN:CA	1:A:1375:GLN:HE21	2.29	0.44
1:D:4260:ASP:OD1	1:D:4262:LYS:CB	2.65	0.44
1:E:5142:GLY:HA2	3:E:5:N LX:C8	2.42	0.44
1:E:5143:GLY:O	1:E:5144:LEU:HB2	2.16	0.44
1:E:5257:LYS:HB2	1:E:5322:VAL:HG12	1.99	0.44
1:F:6214:SER:HA	1:F:6241:HIS:HD2	1.82	0.44
1:G:1090:ASP:HB3	1:G:1093:ALA:HB3	1.97	0.44
1:J:4174:ILE:HG12	1:J:4319:LEU:HD11	1.99	0.44
1:J:4493:SER:O	1:J:4497:MET:HG3	2.16	0.44
1:K:5249:VAL:CB	1:K:5433:VAL:HG21	2.46	0.44
1:A:1199:ARG:HG3	4:A:7447:HOH:O	2.17	0.44
1:B:2216:THR:HG23	1:B:2242:ARG:HB3	1.97	0.44
1:C:3333:GLU:CD	1:C:3333:GLU:H	2.24	0.44
1:D:4225:GLU:O	1:D:4229:VAL:HG23	2.17	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
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:F:6452:ARG:CB	1:F:6465:ILE:HG12	2.44	0.44
1:G:1313:ARG:HG3	1:G:1313:ARG:NH1	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1399:ALA:HB2	1:G:1550:LEU:HD21	1.98	0.44
1:I:3136:MET:HB3	1:I:3218:PHE:CE1	2.52	0.44
1:J:4045:GLN:NE2	1:J:4046:PRO:HD2	2.32	0.44
1:J:4116:CYS:O	1:J:4118:TYR:N	2.51	0.44
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:L:6161:GLU:HG3	1:L:6497:MET:O	2.18	0.44
1:L:6426:PHE:C	1:L:6429:PRO:HD2	2.42	0.44
1:A:1087:CYS:O	1:A:1088:THR:C	2.60	0.44
1:A:1375:GLN:HG2	1:A:1413:LYS:NZ	2.32	0.44
1:C:3353:GLN:NE2	1:C:3465:ILE:H	2.15	0.44
1:G:1049:ILE:HG12	1:G:1122:TYR:CD2	2.52	0.44
1:H:2191:HIS:O	1:H:2195:VAL:HG23	2.18	0.44
1:I:3414:LYS:HD2	1:I:3414:LYS:C	2.42	0.44
1:I:3491:ARG:HB3	1:I:3491:ARG:HH11	1.81	0.44
1:I:3495:MET:O	1:I:3498:LYS:HB2	2.18	0.44
3:I:3:NLX:H203	3:I:3:NLX:O4	2.17	0.44
1:K:5350:ILE:C	1:K:5351:ASN:HD22	2.24	0.44
1:L:6194:GLN:OE1	1:L:6226: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:A:1480:PHE:HZ	1:A:1494:LYS:HG3	1.83	0.44
1:B:2023:PRO:HA	1:B:2024:PRO:HD3	1.87	0.44
1:B:2355:PHE:CE2	1:B:2359:ILE:CG2	2.99	0.44
1:F:6317:PRO:HD3	1:F:6387:PRO:HB2	1.98	0.44
1:F:6501:ALA:O	1:F:6504:ALA:HB3	2.17	0.44
1:G:1086:MET:CE	1:G:1148:ALA:HB2	2.45	0.44
1:G:1101:PHE:CD1	1:G:1472:LEU:HD12	2.52	0.44
1:I:3160:HIS:HE1	1:I:3480:PHE:CE2	2.36	0.44
1:J:4045:GLN:HE21	1:J:4046:PRO:HD2	1.81	0.44
1:J:4220:GLU:O	1:J:4221:SER:HB3	2.18	0.44
1:J:4236:ALA:O	1:J:4237:LYS:C	2.60	0.44
1:K:5246:GLU:HG2	1:K:5447:TYR:OH	2.17	0.44
1:K:5354:GLU:C	1:K:5356:GLY:H	2.25	0.44
1:L:6125:ALA:HB2	1:L:6133:LEU:HD12	1.97	0.44
1:A:1136:MET:HB3	1:A:1218:PHE:CE1	2.53	0.44
1:A:1221:SER:OG	3:A:1:NLX:O1	2.34	0.44
1:A:1319:LEU:H	1:A:1319:LEU:CD1	2.28	0.44
1:B:2437:HIS:HD2	1:B:2444:THR:OG1	2.00	0.44
1:C:3262:LYS:HB3	1:C:3263:PRO:HD3	1.98	0.44
1:E:5241:HIS:HB3	4:E:7347:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:6147:GLY:HA2	4:F:7265:HOH:O	2.17	0.44
1:G:1221:SER:O	1:G:1224:GLY:N	2.49	0.44
1:G:1265:ALA:HB1	1:G:1282:MET:CE	2.48	0.44
1:G:1267:GLN:HA	4:G:7984:HOH:O	2.18	0.44
1:H:2404:LEU:N	1:H:2404:LEU:HD23	2.32	0.44
1:I:3026:VAL:HG23	1:I:3050:PHE:CZ	2.53	0.44
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:K:5354:GLU:O	1:K:5468:HIS:HB2	2.18	0.44
1:L:6126:ASP:O	1:L:6128:THR:N	2.51	0.44
1:A:1064:ARG:O	1:A:1066:THR:HG23	2.18	0.44
1:A:1086:MET:CE	1:A:1110:LEU:HB2	2.39	0.44
1:B:2355:PHE:CD2	1:B:2359:ILE:HD12	2.53	0.44
1:B:2455:PHE:CD2	1:B:2482:LYS:HD3	2.53	0.44
1:C:3126:ASP:C	1:C:3128:THR:H	2.26	0.44
1:F:6087:CYS:O	1:F:6088:THR:C	2.60	0.44
1:G:1191:HIS:HB2	1:G:1327:LEU:HD22	1.99	0.44
1:G:1205:ILE:HD12	1:G:1205:ILE:HA	1.78	0.44
1:H:2064:ARG:NH1	1:H:2294:LEU:HD11	2.33	0.44
1:J:4072:GLU:HG2	4:K:7791:HOH:O	2.17	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:4364:MET:HG3	3:J:4:N LX:H82	1.98	0.44
1:L:6032:LYS:HB2	1:L:6077:VAL:HG22	2.00	0.44
1:L:6185:SER:HB2	1:L:6283:VAL:CG2	2.48	0.44
1:L:6220:GLU:HG2	1:L:6472:LEU:HD21	1.99	0.44
1:A:1394:GLU:CD	1:A:1394:GLU:H	2.24	0.44
1:A:1401:GLU:C	1:A:1403:TYR:H	2.25	0.44
1:B:2285:CYS:HB2	4:B:7947:HOH:O	2.17	0.44
1:D:4132:ARG:HD2	4:D:7062:HOH:O	2.17	0.44
1:D:4258:LYS:HB2	4:D:7713:HOH:O	2.17	0.44
1:E:5179:SER:HB3	1:E:5187:GLY:HA3	1.98	0.44
1:E:5370:GLU:C	1:E:5372:GLN:N	2.75	0.44
1:G:1302:LYS:HB2	1:L:6092:LYS:HZ1	1.83	0.44
1:G:1543:GLU:O	1:G:1547:TRP:HD1	2.00	0.44
1:H:2176:GLY:C	1:H:2189:TRP:HB2	2.43	0.44
1:H:2351:ASN:HD22	1:H:2351:ASN:N	2.16	0.44
1:I:3297:THR:C	1:I:3299:LEU:H	2.25	0.44
1:K:5098:SER:O	1:K:5102:THR:HB	2.17	0.44
1:L:6279:SER:HA	1:L:6282:MET:HE2	1.99	0.44
1:B:2428:VAL:O	1:B:2432:ILE:HG13	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4143:GLY:C	1:D:4145:MET:N	2.75	0.44
1:E:5099:GLU:O	1:E:5102:THR:HG22	2.17	0.44
1:E:5211:ASN:HD22	1:E:5214:SER:HB3	1.82	0.44
1:F:6097:LEU:CB	3:F:6:N LX:H192	2.47	0.44
1:G:1318:LEU:HD12	1:G:1318:LEU:C	2.43	0.44
1:G:1486:SER:C	1:G:1488:GLU:N	2.75	0.44
1:H:2132:ARG:NH1	4:H:7324:HOH:O	2.50	0.44
1:H:2524:GLU:O	1:H:2537:GLN:HA	2.18	0.44
1:I:3140:HIS:CD2	1:I:3147:GLY:HA3	2.53	0.44
1:I:3228:SER:CB	1:I:3250:ALA:H	2.31	0.44
1:I:3257:LYS:HB2	1:I:3322:VAL:HG12	2.00	0.44
1:K:5039:SER:HB3	1:K:5046:PRO:CB	2.48	0.44
1:K:5339:ARG:HB2	1:K:5440:ALA:HA	1.99	0.44
1:K:5527:LEU:HD12	1:K:5528:GLN:H	1.83	0.44
1:A:1463:THR:HG21	1:F:6372:GLN:HB3	2.00	0.44
1:B:2161:GLU:HG3	1:B:2501:ALA:HB2	1.98	0.44
1:B:2536:ALA:C	1:B:2537:GLN:HG3	2.43	0.44
1:G:1252:THR:O	1:G:1253:SER:C	2.61	0.44
1:G:1386:TYR:N	1:G:1387:PRO:HD2	2.33	0.44
1:G:1398:GLU:CD	1:G:1550:LEU:HD13	2.43	0.44
1:I:3344:VAL:HG22	4:I:7956:HOH:O	2.16	0.44
1:J:4236:ALA:O	1:J:4239:LEU:HB2	2.18	0.44
1:K:5235:LEU:HD12	1:K:5327:LEU:CD1	2.40	0.44
1:A:1032:LYS:HD2	1:A:1077:VAL:HG22	2.00	0.43
1:A:1153:ASP:OD2	1:A:1153:ASP:C	2.59	0.43
1:B:2183:GLU:OE2	1:B:2183:GLU:N	2.45	0.43
1:B:2294:LEU:O	1:B:2298:THR:HG23	2.18	0.43
1:C:3065:PHE:C	1:C:3066:THR:CG2	2.91	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:C:3351:ASN:ND2	4:C:7038:HOH:O	2.51	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:D:4242:ARG:HH11	1:D:4242:ARG:CG	2.20	0.43
1:F:6363:LEU:CD1	3:F:6:N LX:H171	2.40	0.43
1:G:1073:PRO:O	1:H:2186:ARG:NH2	2.51	0.43
1:H:2132:ARG:HD2	4:H:7324:HOH:O	2.17	0.43
1:I:3217:ILE:HG13	1:I:3227:VAL:HG13	1.99	0.43
1:I:3271:THR:HG22	1:I:3297:THR:HG23	2.00	0.43
1:I:3461:PRO:HB2	1:I:3464:VAL:HG23	2.00	0.43
1:J:4351:ASN:H	1:J:4354:GLU:CD	2.26	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:6446:MET:HE1	1:L:6539:LEU:HD23	2.00	0.43
1:L:6487:GLU:HB3	4:L:7856:HOH:O	2.17	0.43
1:B:2051:LEU:HD13	1:B:2083:TYR:CE1	2.53	0.43
1:B:2258:LYS:HD2	1:B:2258:LYS:H	1.83	0.43
1:C:3132:ARG:HD3	1:C:3132:ARG:HA	1.78	0.43
1:D:4538:LYS:HB3	1:D:4541:ASP:HB2	1.99	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:G:1153:ASP:OD2	1:G:1153:ASP:C	2.60	0.43
1:G:1237:LYS:O	1:G:1238:ASN:HB2	2.17	0.43
1:H:2143:GLY:N	3:H:2:NLX:H152	2.32	0.43
1:H:2409:ASP:OD2	1:H:2412:LYS:HD2	2.18	0.43
1:H:2420:LEU:CD1	1:H:2547:TRP:CZ2	3.01	0.43
1:I:3199:ARG:NH2	4:I:7409:HOH:O	2.47	0.43
1:I:3480:PHE:HZ	1:I:3494:LYS:HG2	1.82	0.43
1:J:4104:ARG:O	1:J:4482:LYS:NZ	2.51	0.43
1:K:5236:ALA:O	1:K:5237:LYS:C	2.61	0.43
1:L:6093:ALA:HB1	3:L:6:NLX:C19	2.47	0.43
1:L:6186:ARG:NH2	1:L:6326:MET:HE3	2.33	0.43
1:A:1363:LEU:CB	3:A:1:NLX:H91	2.48	0.43
1:B:2105:LYS:HE3	1:B:2483:GLU:OE1	2.19	0.43
1:B:2236:ALA:O	1:B:2237:LYS:C	2.62	0.43
1:C:3200:TRP:O	1:C:3204:ASN:ND2	2.45	0.43
1:C:3264:LEU:CD1	1:C:3316:GLN:HG2	2.47	0.43
1:C:3343:THR:CB	1:C:3442:ALA:HB2	2.40	0.43
1:E:5304:LEU:CD1	3:E:5:NLX:H181	2.34	0.43
1:F:6034:LEU:HD13	1:F:6034:LEU:C	2.44	0.43
1:G:1130:LYS:HE2	1:G:1130:LYS:HB3	1.78	0.43
1:G:1359:ILE:HG23	3:G:1:NLX:H81	1.98	0.43
1:G:1425:MET:HE3	1:G:1426:PHE:CE1	2.45	0.43
1:H:2106:GLU:HA	4:H:7831:HOH:O	2.19	0.43
1:H:2176:GLY:O	1:H:2189:TRP:HB2	2.18	0.43
1:I:3143:GLY:O	1:I:3144:LEU:HB2	2.18	0.43
1:I:3191:HIS:O	1:I:3195:VAL:HG23	2.18	0.43
1:J:4086:MET:HE3	1:J:4112:LEU:CD2	2.49	0.43
1:J:4370:GLU:O	1:J:4372:GLN:HG2	2.18	0.43
1:K:5217:ILE:HD12	1:K:5227:VAL:HG13	2.00	0.43
1:K:5388:LEU:HD22	1:K:5425:MET:CE	2.48	0.43
1:K:5449:PHE:CE2	1:K:5451:TYR:HB3	2.52	0.43
1:A:1064:ARG:NH2	1:A:1114:GLU:OE2	2.49	0.43
1:A:1508:ASN:OD1	1:A:1510:ASN:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2079:ASN:CG	2:B:279:NAG:C1	2.91	0.43
1:B:2309:GLN:HE21	1:B:2309:GLN:C	2.26	0.43
1:B:2408:ASP:HA	1:B:2413:LYS:HE2	2.00	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
1:D:4079:ASN:HB2	2:D:479:NAG:C8	2.48	0.43
1:E:5267:GLN:HG2	1:E:5301:MET:HE1	2.00	0.43
1:F:6143:GLY:C	1:F:6145:MET:N	2.75	0.43
1:G:1138:TRP:O	1:G:1168:ILE:HG12	2.18	0.43
1:G:1266:GLU:O	1:G:1270:ILE:HG13	2.17	0.43
1:G:1403:TYR:CE2	1:G:1420:LEU:HA	2.52	0.43
1:G:1438:ARG:C	1:G:1440:ALA:H	2.26	0.43
1:H:2264:LEU:HD21	1:H:2319:LEU:CD2	2.47	0.43
1:I:3357:TRP:C	1:I:3360:PRO:HD2	2.43	0.43
1:J:4526:TYR:CZ	1:J:4539:LEU:HD13	2.52	0.43
1:L:6143:GLY:O	1:L:6145:MET:HG2	2.18	0.43
1:A:1347:MET:HE3	1:A:1503:PHE:CG	2.53	0.43
1:B:2051:LEU:HD13	1:B:2083:TYR:CD1	2.54	0.43
1:B:2359:ILE:CD1	3:B:2:NLX:H72	2.48	0.43
1:C:3431:VAL:HG21	1:C:3539:LEU:O	2.18	0.43
1:D:4355:PHE:CD2	1:D:4425:MET:HE1	2.54	0.43
1:E:5023:PRO:HB2	1:E:5034:LEU:HD21	2.00	0.43
1:E:5237:LYS:NZ	1:E:5340:ASN:ND2	2.67	0.43
1:E:5420:LEU:C	1:E:5420:LEU:HD23	2.43	0.43
1:F:6153:ASP:C	1:F:6153:ASP:OD2	2.62	0.43
1:G:1352:LYS:HD3	1:G:1450:GLN:NE2	2.33	0.43
1:H:2361:MET:HG2	1:K:5367:PRO:HB3	2.00	0.43
1:I:3034:LEU:HD22	1:I:3034:LEU:C	2.44	0.43
1:I:3262:LYS:HB3	1:I:3263:PRO:HD3	1.99	0.43
1:L:6042:GLY:C	1:L:6043:PHE:CD1	2.97	0.43
1:L:6067:PRO:HG2	4:L:7322:HOH:O	2.18	0.43
1:L:6091:PRO:HB3	1:L:6112:LEU:HD11	1.99	0.43
1:L:6349:GLY:HA3	1:L:6447:TYR:CE2	2.53	0.43
1:L:6447:TYR:C	1:L:6447:TYR:HD2	2.22	0.43
1:B:2220:GLU:OE1	1:B:2221:SER:N	2.52	0.43
1:B:2332:PRO:O	1:B:2336:GLN:HG3	2.18	0.43
1:D:4236:ALA:HA	1:D:4239:LEU:HD12	2.01	0.43
1:D:4252:THR:O	1:D:4252:THR:HG22	2.18	0.43
1:E:5047:VAL:HG21	1:E:5155:LEU:HD23	2.00	0.43
1:E:5153:ASP:OD2	1:E:5155:LEU:HB2	2.19	0.43
1:G:1140:HIS:CE1	1:G:1170:TYR:CE1	3.07	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1220:GLU:O	1:G:1221:SER:HB3	2.19	0.43
1:G:1438:ARG:HH12	1:G:1524:GLU:HG2	1.83	0.43
1:H:2145:MET:HG3	1:H:2304:LEU:HD21	2.00	0.43
1:I:3155:LEU:HD23	1:I:3155:LEU:O	2.19	0.43
1:I:3364:MET:CE	3:I:3:N LX:H171	2.49	0.43
1:J:4233:SER:HA	1:J:4234:PRO:HD3	1.89	0.43
1:J:4239:LEU:HA	1:J:4239:LEU:HD23	1.73	0.43
1:K:5527:LEU:HG	1:K:5529:ILE:CG1	2.49	0.43
1:L:6336:GLN:HE22	1:L:6433:VAL:HA	1.83	0.43
1:L:6366:TYR:HA	1:L:6367:PRO:HD3	1.75	0.43
1:A:1119:LEU:HD12	1:A:1119:LEU:C	2.44	0.43
1:B:2139:ILE:O	1:B:2223:GLY:HA3	2.19	0.43
1:B:2402:LYS:HG2	1:B:2546:PHE:CZ	2.54	0.43
1:B:2414:LYS:HE2	1:B:2414:LYS:HB3	1.86	0.43
1:B:2536:ALA:O	1:B:2537:GLN:HG3	2.18	0.43
1:C:3025:VAL:HG22	1:C:3034:LEU:HD23	2.00	0.43
1:C:3435:ARG:NH2	4:C:7404:HOH:O	2.40	0.43
1:E:5468:HIS:NE2	3:E:5:N LX:O3	2.51	0.43
1:G:1252:THR:HG23	1:G:1425:MET:O	2.18	0.43
1:H:2138:TRP:CZ3	1:H:2219:GLY:HA2	2.53	0.43
1:I:3090:ASP:HB3	1:I:3093:ALA:HB3	1.98	0.43
1:I:3317:PRO:HB3	4:I:7891:HOH:O	2.17	0.43
1:I:3354:GLU:O	1:I:3468:HIS:HB2	2.17	0.43
1:J:4140:HIS:HD2	1:J:4147:GLY:HA3	1.83	0.43
1:J:4185:SER:HB2	1:J:4283:VAL:HG21	2.00	0.43
1:L:6064:ARG:NH1	1:L:6286:LEU:O	2.52	0.43
1:L:6237:LYS:HG3	1:L:6238:ASN:ND2	2.34	0.43
1:A:1412:LYS:O	1:A:1416:LEU:HB2	2.19	0.43
1:A:1445:TYR:OH	1:A:1508:ASN:ND2	2.51	0.43
1:B:2355:PHE:HA	1:B:2359:ILE:HD12	2.01	0.43
1:C:3318:LEU:HD11	3:C:3:N LX:C16	2.48	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:F:6324:ASP:OD2	1:F:6327:LEU:HB3	2.19	0.43
1:G:1252:THR:HG22	1:G:1254:VAL:HG12	2.01	0.43
1:G:1304:LEU:HD13	1:G:1317:PRO:O	2.19	0.43
1:G:1384:LYS:O	1:G:1387:PRO:HD2	2.19	0.43
1:G:1396:ILE:HB	1:G:1397:PRO:CD	2.38	0.43
1:G:1528:GLN:HB2	1:G:1534:GLN:NE2	2.34	0.43
1:H:2447:TYR:C	1:H:2447:TYR:CD2	2.96	0.43
1:I:3318:LEU:HD11	3:I:3:N LX:H101	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:4353:GLN:HE22	1:J:4465:ILE:H	1.67	0.43
1:J:4452:ARG:HG2	1:J:4452:ARG:HH11	1.83	0.43
1:L:6363:LEU:HD22	3:L:6:N LX:H201	2.01	0.43
1:A:1218:PHE:HB2	1:A:1244:ILE:HB	1.99	0.43
1:A:1257:LYS:HD2	1:A:1320:GLY:N	2.30	0.43
1:B:2463:THR:HG23	4:B:7799:HOH:O	2.18	0.43
1:D:4257:LYS:NZ	1:D:4316:GLN:HG3	2.28	0.43
1:E:5329:LEU:HD12	1:E:5329:LEU:N	2.33	0.43
1:F:6358:LEU:HD23	1:F:6468:HIS:HB3	2.00	0.43
1:G:1308:LEU:HD21	1:G:1367:PRO:HG3	2.01	0.43
1:H:2303:PHE:CD2	1:H:2318:LEU:HA	2.53	0.43
1:I:3206:ALA:HA	1:I:3210:GLY:O	2.19	0.43
1:L:6145:MET:CB	1:L:6304:LEU:HD11	2.49	0.43
1:A:1104:ARG:HG2	1:A:1104:ARG:NH1	2.33	0.43
1:C:3447:TYR:HA	1:C:3527:LEU:O	2.19	0.43
1:E:5064:ARG:O	1:E:5065:PHE:HB2	2.19	0.43
1:F:6145:MET:HE2	1:F:6303:PHE:CB	2.49	0.43
1:G:1523:LYS:HD3	1:G:1537:GLN:HE22	1.84	0.43
1:I:3227:VAL:O	1:I:3231:VAL:HG23	2.19	0.43
1:I:3364:MET:CE	3:I:3:N LX:H201	2.47	0.43
1:I:3480:PHE:HZ	1:I:3494:LYS:CG	2.32	0.43
1:J:4407:THR:HG21	1:J:4412:LYS:CD	2.47	0.43
1:A:1330:LYS:HB2	1:A:1335:LEU:HD21	2.01	0.42
1:B:2174:ILE:HD12	1:B:2298:THR:CG2	2.49	0.42
1:B:2290:THR:OG1	1:B:2293:GLU:HG3	2.19	0.42
1:B:2477:GLY:HA2	1:B:2493:SER:OG	2.19	0.42
1:B:2495:MET:HE3	1:B:2499:PHE:HE1	1.82	0.42
1:C:3023:PRO:HA	1:C:3024:PRO:HD3	1.78	0.42
1:C:3044:ALA:O	1:C:3046:PRO:HD3	2.19	0.42
1:E:5218:PHE:HB3	1:E:5244:ILE:HB	1.99	0.42
1:F:6351:ASN:HD22	1:F:6351:ASN:N	2.16	0.42
1:G:1119:LEU:HD12	1:G:1119:LEU:O	2.19	0.42
1:G:1145:MET:HE1	1:G:1303:PHE:HD1	1.84	0.42
1:G:1351:ASN:HD22	1:G:1351:ASN:N	2.16	0.42
1:G:1360:PRO:HB2	4:G:7264:HOH:O	2.19	0.42
1:H:2341:PHE:HE1	1:H:2437:HIS:ND1	2.17	0.42
1:K:5119:LEU:HD12	1:K:5119:LEU:C	2.44	0.42
1:L:6142:GLY:O	3:L:6:N LX:H101	2.18	0.42
1:B:2027:ASP:OD2	1:B:2032:LYS:NZ	2.52	0.42
1:B:2464:VAL:C	1:B:2465:ILE:HD12	2.44	0.42
1:C:3242:ARG:NH1	1:C:3242:ARG:CG	2.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:5518:PRO:HD3	1:E:5535:ALA:HB2	2.01	0.42
1:F:6125:ALA:HB2	1:F:6133:LEU:CD1	2.49	0.42
1:F:6143:GLY:O	1:F:6144:LEU:HB2	2.20	0.42
1:H:2491:ARG:HG2	1:H:2491:ARG:HH11	1.84	0.42
1:I:3104:ARG:HG2	1:I:3104:ARG:HH11	1.84	0.42
1:I:3272:ALA:O	1:I:3289:LYS:HE3	2.19	0.42
1:I:3420:LEU:HD13	1:I:3547:TRP:HZ2	1.81	0.42
1:J:4125:ALA:HB2	1:J:4133:LEU:HD12	2.00	0.42
1:K:5057:LYS:HB3	1:K:5069:GLN:HB2	2.01	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:L:6264:LEU:HD22	1:L:6268:ILE:HD13	2.01	0.42
1:L:6338:GLU:O	1:L:6339:ARG:C	2.63	0.42
1:A:1304:LEU:CG	3:A:1:NLX:H151	2.49	0.42
1:B:2257:LYS:HE2	1:B:2316:GLN:HE22	1.84	0.42
1:D:4267:GLN:HG2	1:D:4301:MET:HE1	2.00	0.42
1:D:4394:GLU:CD	1:D:4394:GLU:H	2.27	0.42
1:E:5359:ILE:HB	1:E:5360:PRO:CD	2.50	0.42
1:G:1104:ARG:HD2	1:G:1108:ILE:HG12	2.00	0.42
1:G:1383:TRP:HA	1:G:1383:TRP:CE3	2.54	0.42
1:H:2389:VAL:HB	1:H:2424:VAL:HG11	2.00	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:A:1098:SER:O	1:A:1102:THR:HB	2.20	0.42
1:A:1358:LEU:C	1:A:1363:LEU:HD12	2.44	0.42
1:A:1467:ASP:N	1:A:1470:ASP:OD2	2.52	0.42
1:B:2252:THR:HG22	1:B:2254:VAL:HG12	2.01	0.42
1:B:2277:THR:HG22	1:B:2278:THR:HG23	2.01	0.42
1:B:2308:LEU:HD11	1:B:2367:PRO:CG	2.49	0.42
1:B:2309:GLN:C	1:B:2309:GLN:NE2	2.77	0.42
1:B:2467:ASP:OD1	1:B:2468:HIS:N	2.46	0.42
1:D:4432:ILE:O	1:D:4433:VAL:C	2.62	0.42
1:E:5126:ASP:O	1:E:5128:THR:N	2.53	0.42
1:E:5211:ASN:HD22	1:E:5214:SER:CB	2.32	0.42
1:E:5304:LEU:HD22	3:E:5:NLX:C10	2.41	0.42
1:E:5309:GLN:NE2	4:E:7812:HOH:O	2.49	0.42
1:F:6097:LEU:HD23	1:F:6146:VAL:HG23	2.00	0.42
1:G:1220:GLU:OE2	1:G:1468:HIS:NE2	2.53	0.42
1:H:2026:VAL:HG12	1:H:2027:ASP:N	2.34	0.42
1:H:2040:LEU:HD13	1:H:2155:LEU:HD13	2.01	0.42
1:H:2404:LEU:HB3	1:H:2413:LYS:CG	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:3257:LYS:HZ3	1:I:3316:GLN:CG	2.33	0.42
1:J:4321:THR:HG22	1:J:4322:VAL:N	2.35	0.42
1:J:4374:ASP:O	1:J:4376:LYS:N	2.52	0.42
1:K:5336:GLN:HE22	1:K:5433:VAL:HA	1.84	0.42
1:L:6188:ASN:ND2	1:L:6324:ASP:OD2	2.52	0.42
1:L:6246:GLU:HG2	1:L:6447:TYR:OH	2.20	0.42
1:A:1175:TRP:CZ2	1:A:1294:LEU:HB2	2.54	0.42
1:A:1404:LEU:O	1:A:1413:LYS:HE2	2.19	0.42
1:A:1426:PHE:CD1	1:A:1426:PHE:N	2.87	0.42
1:A:1527:LEU:HD11	1:A:1533:THR:HG23	2.00	0.42
1:B:2086:MET:HE3	1:B:2112:LEU:HD23	2.02	0.42
1:C:3022:SER:N	4:C:7654:HOH:O	2.51	0.42
1:C:3140:HIS:CD2	1:C:3147:GLY:HA3	2.54	0.42
1:C:3152:TYR:CD1	1:C:3152:TYR:N	2.88	0.42
1:C:3211:ASN:HA	1:C:3212:PRO:HD2	1.93	0.42
1:D:4079:ASN:CB	2:D:479:NAG:H82	2.49	0.42
1:D:4139:ILE:HG12	1:D:4168:ILE:HD11	2.01	0.42
1:D:4164:VAL:HG11	1:D:4205:ILE:HD11	2.01	0.42
1:E:5382:LEU:O	1:E:5385:SER:HB2	2.19	0.42
1:F:6023:PRO:HA	1:F:6024:PRO:HD3	1.74	0.42
1:F:6108:ILE:HA	1:F:6109:PRO:HD3	1.81	0.42
1:G:1521:ASN:O	1:G:1522:GLN:C	2.62	0.42
1:H:2152:TYR:CD1	1:H:2152:TYR:N	2.88	0.42
1:H:2330:LYS:HB3	1:H:2334:GLU:OE2	2.19	0.42
1:J:4132:ARG:HD3	1:J:4132:ARG:HA	1.79	0.42
1:J:4231:VAL:O	1:J:4231:VAL:HG12	2.19	0.42
1:J:4363:LEU:HD22	3:J:4:N LX:C19	2.49	0.42
1:J:4480:PHE:HZ	1:J:4494:LYS:HG3	1.83	0.42
1:K:5025:VAL:CG2	1:K:5034:LEU:HD23	2.50	0.42
1:L:6085:PRO:HG2	1:L:6115:ASP:O	2.19	0.42
1:L:6096:LEU:HD12	1:L:6096:LEU:O	2.19	0.42
1:A:1025:VAL:CG2	1:A:1034:LEU:HD23	2.33	0.42
1:A:1176:GLY:HA2	1:A:1189:TRP:HB2	2.02	0.42
1:A:1420:LEU:HD12	1:A:1547:TRP:HZ2	1.84	0.42
1:A:1421:ILE:H	1:A:1421:ILE:HD12	1.85	0.42
1:B:2104:ARG:CZ	1:B:2108:ILE:HD12	2.50	0.42
1:D:4086:MET:SD	1:D:4089:GLN:NE2	2.92	0.42
1:D:4145:MET:HB3	1:D:4304:LEU:HD21	2.00	0.42
1:E:5447:TYR:HB3	1:E:5517:TRP:CZ2	2.54	0.42
1:F:6492:LEU:O	1:F:6496:VAL:HG23	2.20	0.42
1:G:1372:GLN:HE22	1:L:6463:THR:HB	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:2119:LEU:O	1:H:2119:LEU:HD12	2.19	0.42
1:J:4102:THR:OG1	1:J:4103:ASN:N	2.52	0.42
1:J:4190:GLY:O	1:J:4194:GLN:HG3	2.19	0.42
1:J:4275:LYS:NZ	4:J:7504:HOH:O	2.52	0.42
1:K:5197:ALA:O	1:K:5200:TRP:HB3	2.19	0.42
1:L:6040:LEU:HD13	1:L:6155:LEU:HD13	2.01	0.42
1:L:6097:LEU:HD13	3:L:6:N LX:O4	2.19	0.42
1:L:6297:THR:O	1:L:6298:THR:C	2.63	0.42
1:L:6358:LEU:CD1	1:L:6363:LEU:HD11	2.50	0.42
1:A:1136:MET:HE1	1:A:1500:TRP:HB3	2.00	0.42
1:B:2257:LYS:N	1:B:2257:LYS:HD2	2.34	0.42
1:D:4366:TYR:HA	1:D:4367:PRO:HD3	1.88	0.42
1:F:6086:MET:HB3	1:F:6110:LEU:HD13	2.00	0.42
1:F:6385:SER:O	1:F:6386:TYR:C	2.63	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:H:2404:LEU:O	1:H:2413:LYS:HE2	2.20	0.42
1:I:3138:TRP:CZ3	1:I:3219:GLY:HA2	2.55	0.42
1:I:3286:LEU:C	1:I:3288:GLN:N	2.78	0.42
1:I:3332:PRO:O	1:I:3336:GLN:HG3	2.19	0.42
1:J:4517:TRP:HA	1:J:4518:PRO:HD2	1.91	0.42
1:L:6420:LEU:O	1:L:6421:ILE:C	2.63	0.42
1:L:6452:ARG:HB2	1:L:6465:ILE:HA	2.02	0.42
1:A:1436:ASN:O	1:A:1437:HIS:C	2.63	0.42
1:B:2402:LYS:HE2	1:B:2546:PHE:CD1	2.54	0.42
1:E:5142:GLY:CA	3:E:5:N LX:H82	2.42	0.42
1:E:5414:LYS:NZ	1:E:5414:LYS:HB3	2.34	0.42
1:F:6420:LEU:CD1	1:F:6547:TRP:CZ2	3.02	0.42
1:H:2255:LEU:HD23	1:H:2318:LEU:HD21	2.01	0.42
1:H:2316:GLN:HA	1:H:2317:PRO:HD2	1.91	0.42
1:H:2382:LEU:HA	1:H:2385:SER:OG	2.19	0.42
1:I:3126:ASP:OD1	1:I:3129:LYS:HG3	2.20	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:J:4107:ASN:ND2	1:J:4108:ILE:N	2.68	0.42
1:K:5061:GLY:HA3	1:K:5062:PRO:HD3	1.79	0.42
1:K:5395:LEU:HD13	1:K:5550:LEU:CD2	2.50	0.42
1:L:6105:LYS:HB2	1:L:6481:LEU:O	2.19	0.42
1:L:6268:ILE:CD1	1:L:6301:MET:HE2	2.49	0.42
1:L:6344:VAL:O	1:L:6345:PRO:C	2.61	0.42
1:C:3343:THR:HB	1:C:3442:ALA:CB	2.42	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:5526:TYR:CE2	1:E:5539:LEU:HB2	2.55	0.42
1:F:6190:GLY:O	1:F:6193:ASP:HB2	2.20	0.42
1:G:1223:GLY:O	1:G:1227:VAL:HG23	2.19	0.42
1:H:2190:GLY:O	1:H:2194:GLN:HG3	2.19	0.42
1:I:3298:THR:HG22	1:I:3298:THR:O	2.20	0.42
1:I:3410:THR:HA	1:I:3413:LYS:HB2	2.01	0.42
1:I:3499:PHE:HD2	1:I:3509:PRO:O	2.03	0.42
1:J:4130:LYS:HE2	1:J:4132:ARG:HE	1.83	0.42
1:J:4188:ASN:HD22	1:J:4324:ASP:CG	2.28	0.42
1:K:5420:LEU:O	1:K:5424:VAL:HG23	2.20	0.42
1:L:6171:ARG:HD2	1:L:6175:TRP:O	2.20	0.42
1:L:6375:GLN:HG3	1:L:6400:THR:CG2	2.50	0.42
1:A:1246:GLU:HG2	1:A:1447:TYR:OH	2.19	0.42
1:A:1324:ASP:OD2	1:A:1325:GLY:N	2.52	0.42
1:A:1375:GLN:NE2	1:A:1375:GLN:HA	2.35	0.42
1:C:3218:PHE:CB	1:C:3244:ILE:HB	2.49	0.42
1:C:3444:THR:HG22	1:C:3445:TYR:N	2.35	0.42
1:D:4198:LEU:HD23	1:D:4198:LEU:HA	1.84	0.42
1:E:5537:GLN:NE2	4:E:7903:HOH:O	2.51	0.42
1:F:6243:ALA:O	1:F:6346:TYR:HA	2.19	0.42
1:F:6398:GLU:HB2	4:F:7899:HOH:O	2.18	0.42
1:G:1551:PHE:C	1:G:1553:LYS:H	2.28	0.42
1:H:2304:LEU:CG	3:H:2:NLX:H201	2.49	0.42
1:H:2311:ASP:HB3	1:H:2314:GLU:CG	2.50	0.42
1:K:5069:GLN:HA	1:K:5069:GLN:HE21	1.83	0.42
1:L:6126:ASP:C	1:L:6128:THR:H	2.28	0.42
1:L:6545:ALA:HA	1:L:6548:THR:CG2	2.49	0.42
1:A:1049:ILE:HD13	1:A:1122:TYR:CE2	2.55	0.41
1:A:1218:PHE:HA	1:A:1244:ILE:O	2.20	0.41
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:C:3512:GLU:HB3	4:C:7492:HOH:O	2.19	0.41
1:E:5202:GLN:HG2	4:E:7074:HOH:O	2.19	0.41
1:F:6064:ARG:HH11	1:F:6287:ARG:HA	1.84	0.41
1:F:6453:PRO:HA	1:F:6489:GLU:OE1	2.20	0.41
1:G:1251:LEU:HB2	1:G:1429:PRO:HB3	2.00	0.41
1:G:1264:LEU:HD11	1:G:1316:GLN:HG2	2.02	0.41
1:I:3414:LYS:HD2	1:I:3414:LYS:O	2.20	0.41
1:I:3534:GLN:CD	1:I:3534:GLN:N	2.78	0.41
1:J:4527:LEU:HD11	1:J:4533:THR:HG22	2.02	0.41
1:K:5136:MET:HE3	1:K:5504:ALA:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:5241:HIS:O	1:K:5345:PRO:HD2	2.20	0.41
1:L:6111:LYS:NZ	4:L:7632:HOH:O	2.49	0.41
1:A:1303:PHE:CZ	1:A:1319:LEU:HD11	2.55	0.41
1:A:1331:THR:O	1:A:1332:PRO:C	2.63	0.41
1:A:1363:LEU:HD22	3:A:1:NLX:C18	2.43	0.41
1:E:5225:GLU:O	1:E:5228:SER:HB3	2.19	0.41
1:F:6218:PHE:CB	1:F:6244:ILE:HB	2.50	0.41
1:F:6262:LYS:HD2	1:F:6262:LYS:HA	1.90	0.41
1:F:6420:LEU:CD1	1:F:6547:TRP:HZ2	2.33	0.41
1:F:6445:TYR:CE1	1:F:6509:PRO:HD2	2.55	0.41
1:G:1381:LEU:HD21	1:L:6459:MET:HB3	2.01	0.41
1:G:1398:GLU:OE1	1:G:1550:LEU:HD13	2.20	0.41
1:G:1519:GLU:O	1:G:1520:TYR:C	2.62	0.41
1:H:2304:LEU:HD22	3:H:2:NLX:H162	2.00	0.41
1:I:3023:PRO:HA	1:I:3024:PRO:HD3	1.68	0.41
1:I:3091:PRO:HB3	1:I:3112:LEU:HD11	2.02	0.41
1:I:3251:LEU:HD12	1:I:3433:VAL:HG22	2.02	0.41
1:J:4333:GLU:CD	1:J:4333:GLU:N	2.75	0.41
1:K:5333:GLU:OE1	1:K:5333:GLU:N	2.31	0.41
1:K:5438:ARG:HD2	1:K:5522:GLN:NE2	2.35	0.41
1:K:5493:SER:O	1:K:5497:MET:HG3	2.20	0.41
1:L:6254:VAL:HG12	4:L:7486:HOH:O	2.19	0.41
1:L:6420:LEU:HD11	1:L:6547:TRP:CH2	2.55	0.41
1:A:1246:GLU:HB3	1:A:1471:GLU:OE1	2.20	0.41
1:A:1526:TYR:CZ	1:A:1536:ALA:HB3	2.55	0.41
1:D:4317:PRO:O	1:D:4318:LEU:HB3	2.20	0.41
1:E:5221:SER:HB2	3:E:5:NLX:O3	2.19	0.41
1:E:5372:GLN:HB3	1:E:5410:THR:OG1	2.20	0.41
1:F:6534:GLN:CD	1:F:6534:GLN:N	2.78	0.41
1:G:1145:MET:CG	1:G:1304:LEU:HD21	2.50	0.41
1:G:1145:MET:HE3	1:G:1145:MET:HB3	1.89	0.41
1:G:1244:ILE:HD11	1:G:1503:PHE:CD2	2.55	0.41
1:G:1367:PRO:O	1:G:1368:LEU:HD23	2.20	0.41
1:G:1377:THR:O	1:G:1378:ALA:C	2.63	0.41
1:G:1435:ARG:NH2	1:G:1541:ASP:OD2	2.53	0.41
1:H:2142:GLY:C	3:H:2:NLX:H152	2.45	0.41
1:H:2368:LEU:O	1:K:5368:LEU:O	2.38	0.41
1:I:3155:LEU:C	1:I:3155:LEU:CD2	2.94	0.41
1:I:3220:GLU:HA	1:I:3246:GLU:O	2.20	0.41
1:K:5051:LEU:HD22	1:K:5083:TYR:CE1	2.55	0.41
1:K:5340:ASN:O	1:K:5340:ASN:CG	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:K:5540:LYS:HA	1:K:5543:GLU:OE2	2.21	0.41
1:L:6383:TRP:HA	1:L:6383:TRP:CE3	2.55	0.41
1:B:2237:LYS:HD3	1:B:2237:LYS:HA	1.89	0.41
1:C:3304:LEU:HA	3:C:3:NLX:H201	2.02	0.41
1:C:3348:VAL:O	1:C:3446:MET:HA	2.20	0.41
1:C:3366:TYR:HA	1:C:3367:PRO:HD3	1.79	0.41
1:D:4351:ASN:ND2	1:D:4449:PHE:HB3	2.35	0.41
1:D:4486:SER:HB2	1:D:4489:GLU:H	1.84	0.41
1:E:5487:GLU:HG3	1:E:5491:ARG:CZ	2.50	0.41
1:G:1170:TYR:CD1	1:G:1170:TYR:N	2.89	0.41
1:G:1448:GLU:OE2	1:G:1539:LEU:CD1	2.69	0.41
1:H:2176:GLY:O	1:H:2189:TRP:N	2.53	0.41
1:J:4296:GLU:O	1:J:4300:LYS:HG3	2.20	0.41
1:J:4524:GLU:HG3	1:J:4538:LYS:CE	2.50	0.41
1:K:5140:HIS:CD2	1:K:5140:HIS:C	2.98	0.41
1:K:5255:LEU:O	1:K:5320:GLY:HA3	2.21	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:L:6412:LYS:O	1:L:6416:LEU:HD12	2.20	0.41
1:B:2161:GLU:HG3	1:B:2501:ALA:CB	2.51	0.41
1:B:2423:ASP:HA	4:B:7059:HOH:O	2.19	0.41
1:C:3104:ARG:NH1	1:C:3153:ASP:HB2	2.36	0.41
1:D:4252:THR:O	1:D:4253:SER:C	2.63	0.41
1:D:4442:ALA:HA	1:D:4443:PRO:HD3	1.87	0.41
1:E:5290:THR:HG23	1:E:5293:GLU:OE2	2.21	0.41
1:F:6492:LEU:HD12	1:F:6495:MET:HE2	2.02	0.41
1:G:1045:GLN:NE2	1:G:1046:PRO:HD2	2.35	0.41
1:G:1345:PRO:HA	1:G:1443:PRO:O	2.21	0.41
1:G:1452:ARG:HA	1:G:1453:PRO:HD2	1.85	0.41
1:H:2345:PRO:HA	1:H:2443:PRO:O	2.20	0.41
1:I:3389:VAL:HG23	1:I:3391:ILE:HG13	2.03	0.41
1:K:5104:ARG:O	1:K:5482:LYS:NZ	2.39	0.41
1:L:6093:ALA:CB	3:L:6:NLX:H192	2.50	0.41
1:L:6363:LEU:CB	3:L:6:NLX:H162	2.48	0.41
1:A:1186:ARG:HB3	1:A:1324:ASP:HB2	2.03	0.41
1:A:1398:GLU:OE2	1:A:1550:LEU:HD13	2.20	0.41
1:D:4279:SER:O	1:D:4283:VAL:HG23	2.21	0.41
1:E:5034:LEU:C	1:E:5034:LEU:HD22	2.45	0.41
1:E:5153:ASP:OD2	1:E:5153:ASP:C	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:6047:VAL:HG21	1:F:6155:LEU:CD2	2.48	0.41
1:F:6096:LEU:HD23	1:F:6363:LEU:HD21	2.03	0.41
1:F:6268:ILE:O	1:F:6269:ALA:C	2.63	0.41
1:H:2074:TRP:CE2	1:H:2078:LYS:HD2	2.55	0.41
1:H:2097:LEU:CD1	3:H:2:N LX:H11	2.51	0.41
1:H:2354:GLU:O	1:H:2468:HIS:HB2	2.20	0.41
1:I:3289:LYS:HA	1:I:3293:GLU:OE2	2.20	0.41
1:I:3304:LEU:HA	3:I:3:N LX:H202	2.01	0.41
1:I:3364:MET:SD	3:I:3:N LX:H171	2.61	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:L:6160:HIS:CD2	1:L:6497:MET:HE1	2.55	0.41
1:L:6311:ASP:OD1	1:L:6313:ARG:N	2.49	0.41
1:A:1373:LEU:HD12	1:A:1373:LEU:N	2.36	0.41
1:A:1447:TYR:HB3	1:A:1517:TRP:CZ2	2.55	0.41
1:C:3355:PHE:CD1	1:C:3421:ILE:HG21	2.56	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:D:4145:MET:CB	1:D:4304:LEU:HD21	2.51	0.41
1:D:4275:LYS:HD3	1:D:4275:LYS:HA	1.73	0.41
1:D:4325:GLY:O	1:D:4329:LEU:CD2	2.69	0.41
1:E:5447:TYR:C	1:E:5447:TYR:CD2	2.98	0.41
1:F:6370:GLU:C	1:F:6372:GLN:H	2.27	0.41
1:H:2027:ASP:CG	1:H:2032:LYS:NZ	2.79	0.41
1:H:2103:ASN:O	1:H:2481:LEU:HB2	2.21	0.41
1:H:2107:ASN:ND2	1:H:2108:ILE:N	2.68	0.41
1:I:3043:PHE:CD1	1:I:3043:PHE:N	2.88	0.41
1:I:3112:LEU:O	1:I:3113:SER:HB2	2.20	0.41
1:J:4211:ASN:HA	1:J:4212:PRO:HD2	1.94	0.41
1:L:6546:PHE:O	1:L:6549:ASN:HB3	2.20	0.41
1:A:1140:HIS:HD2	1:A:1141:GLY:O	2.03	0.41
1:A:1367:PRO:HB3	1:F:6361:MET:HG2	2.02	0.41
1:A:1420:LEU:HD12	1:A:1547:TRP:CZ2	2.55	0.41
1:B:2381:LEU:O	1:B:2384:LYS:N	2.53	0.41
1:C:3205:ILE:HD12	1:C:3205:ILE:HA	1.95	0.41
1:D:4375:GLN:HE21	1:D:4375:GLN:HB3	1.50	0.41
1:F:6336:GLN:O	1:F:6339:ARG:HD2	2.21	0.41
1:F:6451:TYR:HE2	1:F:6489:GLU:HG3	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1311:ASP:HA	1:G:1312:PRO:HD3	1.90	0.41
1:G:1354:GLU:HA	1:G:1354:GLU:OE1	2.20	0.41
1:H:2358:LEU:HG	1:H:2363:LEU:HD12	2.03	0.41
1:H:2464:VAL:HG12	1:H:2467:ASP:HB2	2.03	0.41
1:I:3498:LYS:HB3	1:I:3514:LEU:CD1	2.47	0.41
1:L:6090:ASP:HB3	1:L:6093:ALA:HB3	2.03	0.41
1:L:6393:LYS:O	1:L:6396:ILE:HG12	2.21	0.41
1:A:1104:ARG:NH1	1:A:1153:ASP:OD1	2.54	0.41
1:A:1126:ASP:OD2	1:A:1129:LYS:HG2	2.21	0.41
1:A:1220:GLU:O	1:A:1221:SER:HB3	2.21	0.41
1:A:1417:PHE:O	1:A:1420:LEU:HB3	2.21	0.41
1:A:1461:PRO:C	1:A:1463:THR:N	2.79	0.41
1:B:2381:LEU:O	1:B:2382:LEU:C	2.64	0.41
1:C:3055:PHE:CE1	1:C:3197:ALA:HB2	2.56	0.41
1:C:3067:PRO:HB3	1:C:3192:LEU:HD13	2.03	0.41
1:C:3143:GLY:CA	3:C:3:NLX:C15	2.94	0.41
1:C:3175:TRP:CZ2	1:C:3294:LEU:HB2	2.56	0.41
1:C:3475:VAL:HG22	1:C:3496:VAL:CG1	2.50	0.41
1:D:4488:GLU:HG2	1:D:4489:GLU:N	2.35	0.41
1:E:5375:GLN:HE22	1:E:5401:GLU:HA	1.85	0.41
1:E:5455:PHE:CE1	1:E:5478:ALA:HB3	2.56	0.41
1:E:5491:ARG:HG2	1:E:5491:ARG:NH1	2.36	0.41
1:F:6241:HIS:C	1:F:6242:ARG:CG	2.94	0.41
1:F:6262:LYS:NZ	1:F:6282:MET:CE	2.84	0.41
1:F:6514:LEU:O	1:F:6515:PRO:C	2.61	0.41
1:G:1132:ARG:HD3	1:G:1132:ARG:HA	1.80	0.41
1:G:1395:LEU:HD22	1:G:1550:LEU:HD12	2.03	0.41
1:G:1402:LYS:O	1:G:1402:LYS:HG3	2.20	0.41
1:G:1428:VAL:CB	1:G:1429:PRO:HD3	2.46	0.41
1:H:2411:VAL:C	1:H:2413:LYS:N	2.77	0.41
1:I:3177:PHE:CD2	1:I:3177:PHE:N	2.89	0.41
1:I:3277:THR:HG22	1:I:3278:THR:HG23	2.03	0.41
1:I:3473:PHE:HB3	1:I:3478:ALA:HB3	2.02	0.41
1:J:4351:ASN:HB3	1:J:4466:GLY:O	2.21	0.41
1:J:4363:LEU:HD22	3:J:4:NLX:C18	2.51	0.41
1:K:5034:LEU:HD13	1:K:5034:LEU:O	2.21	0.41
1:K:5065:PHE:C	1:K:5066:THR:CG2	2.94	0.41
1:K:5217:ILE:HG13	1:K:5227:VAL:HG13	2.03	0.41
1:K:5527:LEU:HG	1:K:5529:ILE:HG13	2.03	0.41
1:L:6055:PHE:CD1	1:L:6055:PHE:C	2.98	0.41
1:L:6140:HIS:CD2	1:L:6141:GLY:N	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:6218:PHE:HB2	1:L:6244:ILE:HB	2.03	0.41
1:L:6304:LEU:HB3	3:L:6:N LX:C17	2.51	0.41
1:L:6375:GLN:O	1:L:6378:ALA:HB3	2.21	0.41
1:L:6444:THR:HG22	1:L:6445:TYR:N	2.35	0.41
1:A:1140:HIS:CD2	1:A:1140:HIS:C	2.99	0.41
1:A:1205:ILE:HD12	1:A:1205:ILE:HA	1.92	0.41
1:A:1494:LYS:O	1:A:1498:LYS:HB2	2.21	0.41
1:B:2331:THR:O	1:B:2332:PRO:C	2.63	0.41
1:C:3104:ARG:HH11	1:C:3104:ARG:HG2	1.86	0.41
1:C:3371:GLY:HA2	1:D:4371:GLY:HA3	2.02	0.41
1:E:5145:MET:CG	1:E:5318:LEU:HD23	2.51	0.41
1:E:5237:LYS:HZ2	1:E:5340:ASN:ND2	2.19	0.41
1:E:5257:LYS:HE3	1:E:5316:GLN:OE1	2.20	0.41
1:E:5493:SER:O	1:E:5497:MET:HG3	2.21	0.41
1:F:6458:ASP:C	1:F:6460:LYS:H	2.29	0.41
1:I:3547:TRP:O	1:I:3548:THR:C	2.64	0.41
1:J:4455:PHE:CE2	1:J:4482:LYS:HB2	2.56	0.41
1:L:6452:ARG:HA	1:L:6453:PRO:HD2	1.95	0.41
3:L:6:N LX:H203	3:L:6:N LX:O4	2.21	0.41
1:B:2549:ASN:O	1:B:2552:ALA:N	2.52	0.40
1:D:4030:HIS:CD2	1:D:4071:ALA:HB3	2.56	0.40
1:D:4057:LYS:HG3	1:D:4058:PRO:HD2	2.03	0.40
1:D:4079:ASN:ND2	4:D:7835:HOH:O	2.48	0.40
1:D:4156:ALA:O	1:D:4157:LEU:C	2.64	0.40
1:D:4309:GLN:CD	1:D:4310:GLY:N	2.79	0.40
1:E:5346:TYR:HB3	1:E:5437:HIS:CD2	2.56	0.40
1:F:6330:LYS:HB2	1:F:6334:GLU:OE1	2.20	0.40
1:F:6359:ILE:HG23	3:F:6:N LX:H161	2.03	0.40
1:F:6391:ILE:O	1:F:6392:ALA:C	2.63	0.40
1:G:1149:ALA:CB	1:G:1169:GLN:HG3	2.51	0.40
1:G:1486:SER:C	1:G:1488:GLU:H	2.29	0.40
1:H:2344:VAL:O	1:H:2345:PRO:C	2.65	0.40
1:H:2435:ARG:O	1:H:2438:ARG:HB3	2.22	0.40
1:I:3107:ASN:HD22	1:I:3108:ILE:H	1.69	0.40
1:I:3354:GLU:HB2	1:I:3422:ALA:HB1	2.04	0.40
1:J:4313:ARG:HG2	1:J:4386:TYR:CE2	2.57	0.40
1:K:5313:ARG:HA	1:K:5386:TYR:CD2	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:L:6452:ARG:HG2	1:L:6452:ARG:NH1	2.36	0.40
1:A:1268:ILE:CG1	1:A:1301:MET:HE2	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:2241:HIS:O	1:B:2242:ARG:HD2	2.21	0.40
1:C:3176:GLY:C	1:C:3177:PHE:CD2	3.00	0.40
1:C:3495:MET:HG3	1:C:3514:LEU:CD2	2.49	0.40
1:D:4338:GLU:H	1:D:4338:GLU:HG3	1.54	0.40
1:D:4370:GLU:HA	1:D:4370:GLU:OE2	2.22	0.40
1:D:4455:PHE:CD2	1:D:4482:LYS:HD3	2.56	0.40
1:E:5385:SER:C	1:E:5387:PRO:HD2	2.46	0.40
1:F:6303:PHE:HB3	1:F:6317:PRO:O	2.21	0.40
1:G:1517:TRP:CE3	1:G:1527:LEU:HD22	2.56	0.40
1:H:2040:LEU:O	1:H:2041:GLU:C	2.64	0.40
1:H:2428:VAL:HB	1:H:2429:PRO:HD3	2.03	0.40
1:J:4138:TRP:CH2	1:J:4220:GLU:HB2	2.57	0.40
1:K:5205:ILE:HD12	1:K:5205:ILE:HA	1.88	0.40
1:L:6104:ARG:HD2	4:L:7255:HOH:O	2.22	0.40
1:A:1123:THR:O	1:A:1123:THR:HG23	2.21	0.40
1:A:1229:VAL:O	1:A:1232:LEU:N	2.51	0.40
1:A:1316:GLN:OE1	1:A:1316:GLN:HA	2.21	0.40
1:B:2205:ILE:HG13	1:B:2210:GLY:HA3	2.02	0.40
1:B:2373:LEU:CD2	1:B:2378:ALA:HB2	2.33	0.40
1:B:2439:ASP:C	1:B:2441:GLY:N	2.80	0.40
1:C:3040:LEU:HD13	1:C:3155:LEU:HD13	2.03	0.40
1:C:3223:GLY:O	1:C:3227:VAL:HG23	2.22	0.40
1:C:3464:VAL:CG2	1:D:4370:GLU:HG3	2.51	0.40
1:E:5221:SER:HA	1:E:5247:SER:O	2.21	0.40
1:F:6074:TRP:NE1	1:F:6078:LYS:HB2	2.36	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:6401:GLU:C	1:F:6403:TYR:N	2.80	0.40
1:G:1221:SER:OG	1:G:1222:ALA:N	2.53	0.40
1:H:2091:PRO:HG3	1:H:2112:LEU:HD11	2.04	0.40
1:H:2264:LEU:HD22	1:H:2316:GLN:HG3	2.02	0.40
1:I:3151:THR:HB	1:I:3152:TYR:CE1	2.55	0.40
1:I:3359:ILE:HG23	3:I:3:NLX:C15	2.51	0.40
1:I:3447:TYR:C	1:I:3447:TYR:HD2	2.29	0.40
1:I:3452:ARG:CZ	1:I:3462:LYS:HA	2.52	0.40
1:J:4061:GLY:HA2	4:J:8043:HOH:O	2.21	0.40
1:J:4318:LEU:HD12	1:J:4318:LEU:C	2.46	0.40
1:K:5318:LEU:HD11	3:K:5:NLX:C2	2.52	0.40
1:K:5357:TRP:O	1:K:5361:MET:CB	2.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:5368:LEU:C	1:K:5370:GLU:H	2.28	0.40
1:K:5425:MET:HG2	4:K:7147:HOH:O	2.22	0.40
1:K:5495:MET:O	1:K:5499:PHE:HB2	2.22	0.40
1:L:6145:MET:HE2	1:L:6303:PHE:HB3	2.02	0.40
1:L:6358:LEU:HD11	1:L:6363:LEU:HD11	2.04	0.40
1:A:1266:GLU:O	1:A:1270:ILE:HD12	2.21	0.40
1:A:1341:PHE:CD2	1:A:1341:PHE:N	2.89	0.40
1:A:1519:GLU:HG2	1:A:1520:TYR:N	2.36	0.40
1:A:1539:LEU:N	4:A:7558:HOH:O	2.54	0.40
1:B:2026:VAL:CG1	1:B:2027:ASP:N	2.84	0.40
1:D:4211:ASN:HA	1:D:4212:PRO:HD2	1.93	0.40
1:E:5022:SER:HB3	4:E:8085:HOH:O	2.21	0.40
1:E:5145:MET:CB	1:E:5304:LEU:HD11	2.49	0.40
1:F:6449:PHE:CE2	1:F:6451:TYR:HB3	2.57	0.40
1:F:6471:GLU:O	1:F:6475:VAL:HG23	2.21	0.40
1:G:1447:TYR:CD2	1:G:1447:TYR:C	3.00	0.40
1:H:2048:ALA:HB3	1:H:2123:THR:CG2	2.47	0.40
1:H:2244:ILE:HG12	1:H:2347:MET:HB3	2.03	0.40
1:I:3191:HIS:HD2	1:I:3321:THR:HG23	1.85	0.40
1:J:4049:ILE:HG12	1:J:4122:TYR:CD2	2.56	0.40
1:J:4182:ASP:N	1:J:4182:ASP:OD2	2.54	0.40
1:K:5450:GLN:O	1:K:5451:TYR:HB2	2.21	0.40
1:K:5498:LYS:HG2	1:K:5502:ASN:ND2	2.33	0.40
1:L:6139:ILE:C	4:L:7115:HOH:O	2.64	0.40
1:L:6263:PRO:HB2	4:L:7197:HOH:O	2.21	0.40
1:L:6351:ASN:N	1:L:6351:ASN:HD22	2.19	0.40
1:L:6384:LYS:C	1:L:6386:TYR:H	2.28	0.40
1:A:1420:LEU:CD1	1:A:1547:TRP:CZ2	3.05	0.40
1:A:1420:LEU:CD1	1:A:1547:TRP:HZ2	2.35	0.40
1:B:2339:ARG:O	1:B:2341:PHE:CD2	2.74	0.40
1:C:3526:TYR:CE1	1:C:3539:LEU:HD13	2.57	0.40
1:F:6185:SER:HB2	1:F:6283:VAL:HG21	2.03	0.40
1:H:2268:ILE:HG12	1:H:2301:MET:HE2	2.03	0.40
1:H:2420:LEU:CD1	1:H:2547:TRP:HZ2	2.33	0.40
1:J:4355:PHE:HB2	1:J:4422:ALA:HB2	2.02	0.40
1:J:4428:VAL:CB	1:J:4429:PRO:HD3	2.43	0.40
1:K:5036:LYS:HG2	1:K:5049:ILE:HB	2.03	0.40
1:K:5142:GLY:CA	3:K:5:N LX:H82	2.52	0.40
1:K:5389:VAL:HB	1:K:5391:ILE:HG13	2.03	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%)	7	26
1	B	530/548 (97%)	476 (90%)	48 (9%)	6 (1%)	11	36
1	C	529/548 (96%)	489 (92%)	33 (6%)	7 (1%)	9	32
1	D	531/548 (97%)	491 (92%)	36 (7%)	4 (1%)	16	44
1	E	529/548 (96%)	482 (91%)	40 (8%)	7 (1%)	9	32
1	F	529/548 (96%)	477 (90%)	44 (8%)	8 (2%)	8	28
1	G	530/548 (97%)	467 (88%)	55 (10%)	8 (2%)	8	28
1	H	529/548 (96%)	470 (89%)	52 (10%)	7 (1%)	9	32
1	I	529/548 (96%)	466 (88%)	56 (11%)	7 (1%)	9	32
1	J	530/548 (97%)	484 (91%)	40 (8%)	6 (1%)	11	36
1	K	529/548 (96%)	475 (90%)	48 (9%)	6 (1%)	11	36
1	L	529/548 (96%)	467 (88%)	53 (10%)	9 (2%)	7	26
All	All	6354/6576 (97%)	5724 (90%)	546 (9%)	84 (1%)	9	32

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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%)	37 71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	448/463 (97%)	432 (96%)	16 (4%)	31	65
1	C	447/463 (96%)	422 (94%)	25 (6%)	19	50
1	D	448/463 (97%)	425 (95%)	23 (5%)	21	53
1	E	447/463 (96%)	426 (95%)	21 (5%)	23	56
1	F	447/463 (96%)	432 (97%)	15 (3%)	32	66
1	G	448/463 (97%)	419 (94%)	29 (6%)	15	44
1	H	447/463 (96%)	429 (96%)	18 (4%)	28	62
1	I	447/463 (96%)	422 (94%)	25 (6%)	19	50
1	J	448/463 (97%)	423 (94%)	25 (6%)	19	50
1	K	447/463 (96%)	423 (95%)	24 (5%)	20	51
1	L	447/463 (96%)	431 (96%)	16 (4%)	31	65
All	All	5369/5556 (97%)	5119 (95%)	250 (5%)	23	56

All (250) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1253	SER
1	A	1264	LEU
1	A	1304	LEU
1	A	1309	GLN
1	A	1319	LEU
1	A	1341	PHE
1	A	1394	GLU
1	A	1408	ASP
1	A	1410	THR
1	A	1416	LEU
1	A	1488	GLU
1	A	1491	ARG
1	A	1498	LYS
1	B	2034	LEU
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

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Mol	Chain	Res	Type
1	B	2341	PHE
1	B	2366	TYR
1	B	2394	GLU
1	B	2404	LEU
1	B	2420	LEU
1	B	2483	GLU
1	B	2512	GLU
1	C	3027	ASP
1	C	3072	GLU
1	C	3088	THR
1	C	3106	GLU
1	C	3137	VAL
1	C	3155	LEU
1	C	3220	GLU
1	C	3221	SER
1	C	3225	GLU
1	C	3242	ARG
1	C	3261	VAL
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	3374	ASP
1	C	3394	GLU
1	C	3414	LYS
1	C	3420	LEU
1	C	3483	GLU
1	C	3534	GLN
1	D	4027	ASP
1	D	4078	LYS
1	D	4106	GLU
1	D	4146	VAL
1	D	4218	PHE
1	D	4242	ARG
1	D	4253	SER
1	D	4264	LEU
1	D	4275	LYS
1	D	4304	LEU

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Mol	Chain	Res	Type
1	D	4309	GLN
1	D	4316	GLN
1	D	4327	LEU
1	D	4338	GLU
1	D	4363	LEU
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	5155	LEU
1	E	5203	ASP
1	E	5205	ILE
1	E	5218	PHE
1	E	5242	ARG
1	E	5258	LYS
1	E	5266	GLU
1	E	5289	LYS
1	E	5292	GLU
1	E	5305	SER
1	E	5319	LEU
1	E	5340	ASN
1	E	5370	GLU
1	E	5394	GLU
1	E	5408	ASP
1	E	5414	LYS
1	E	5463	THR
1	F	6072	GLU
1	F	6155	LEU
1	F	6214	SER
1	F	6221	SER
1	F	6249	VAL
1	F	6257	LYS
1	F	6258	LYS
1	F	6264	LEU

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Mol	Chain	Res	Type
1	F	6277	THR
1	F	6299	LEU
1	F	6323	ILE
1	F	6374	ASP
1	F	6471	GLU
1	F	6534	GLN
1	F	6541	ASP
1	G	1034	LEU
1	G	1041	GLU
1	G	1104	ARG
1	G	1105	LYS
1	G	1128	THR
1	G	1146	VAL
1	G	1205	ILE
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	1304	LEU
1	G	1309	GLN
1	G	1319	LEU
1	G	1366	TYR
1	G	1375	GLN
1	G	1380	SER
1	G	1398	GLU
1	G	1407	THR
1	G	1458	ASP
1	G	1463	THR
1	G	1500	TRP
1	G	1519	GLU
1	G	1522	GLN
1	G	1541	ASP
1	H	2034	LEU
1	H	2111	LYS
1	H	2129	LYS
1	H	2132	ARG
1	H	2155	LEU
1	H	2225	GLU

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Mol	Chain	Res	Type
1	H	2258	LYS
1	H	2292	GLU
1	H	2299	LEU
1	H	2309	GLN
1	H	2338	GLU
1	H	2342	HIS
1	H	2404	LEU
1	H	2409	ASP
1	H	2411	VAL
1	H	2479	PRO
1	H	2483	GLU
1	H	2500	TRP
1	I	3033	VAL
1	I	3034	LEU
1	I	3064	ARG
1	I	3072	GLU
1	I	3105	LYS
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	3372	GLN
1	I	3374	ASP
1	I	3385	SER
1	I	3414	LYS
1	I	3420	LEU
1	I	3447	TYR
1	I	3512	GLU
1	I	3534	GLN
1	J	4034	LEU
1	J	4041	GLU
1	J	4072	GLU
1	J	4102	THR
1	J	4104	ARG

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Mol	Chain	Res	Type
1	J	4130	LYS
1	J	4205	ILE
1	J	4218	PHE
1	J	4258	LYS
1	J	4261	VAL
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	4463	THR
1	J	4471	GLU
1	J	4506	ASN
1	J	4519	GLU
1	K	5033	VAL
1	K	5034	LEU
1	K	5066	THR
1	K	5069	GLN
1	K	5086	MET
1	K	5128	THR
1	K	5155	LEU
1	K	5220	GLU
1	K	5225	GLU
1	K	5240	PHE
1	K	5258	LYS
1	K	5292	GLU
1	K	5299	LEU
1	K	5305	SER
1	K	5309	GLN
1	K	5330	LYS
1	K	5338	GLU
1	K	5341	PHE
1	K	5374	ASP
1	K	5375	GLN
1	K	5390	CYS
1	K	5463	THR

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Mol	Chain	Res	Type
1	K	5499	PHE
1	K	5512	GLU
1	L	6034	LEU
1	L	6088	THR
1	L	6130	LYS
1	L	6155	LEU
1	L	6205	ILE
1	L	6218	PHE
1	L	6220	GLU
1	L	6247	SER
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	6463	THR
1	L	6500	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (199) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1030	HIS
1	A	1079	ASN
1	A	1095	GLN
1	A	1107	ASN
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
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

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Mol	Chain	Res	Type
1	A	1502	ASN
1	B	2045	GLN
1	B	2069	GLN
1	B	2079	ASN
1	B	2107	ASN
1	B	2140	HIS
1	B	2162	ASN
1	B	2184	HIS
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	2532	ASN
1	B	2537	GLN
1	C	3069	GLN
1	C	3095	GLN
1	C	3107	ASN
1	C	3140	HIS
1	C	3162	ASN
1	C	3238	ASN
1	C	3241	HIS
1	C	3336	GLN
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	3516	HIS
1	C	3532	ASN
1	C	3534	GLN
1	C	3537	GLN
1	D	4030	HIS
1	D	4045	GLN
1	D	4069	GLN
1	D	4107	ASN
1	D	4131	ASN
1	D	4140	HIS

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Mol	Chain	Res	Type
1	D	4241	HIS
1	D	4309	GLN
1	D	4336	GLN
1	D	4351	ASN
1	D	4353	GLN
1	D	4372	GLN
1	D	4375	GLN
1	D	4436	ASN
1	D	4450	GLN
1	D	4508	ASN
1	D	4510	ASN
1	D	4516	HIS
1	D	4528	GLN
1	D	4534	GLN
1	D	4537	GLN
1	E	5079	ASN
1	E	5107	ASN
1	E	5131	ASN
1	E	5140	HIS
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	5436	ASN
1	E	5437	HIS
1	E	5532	ASN
1	E	5537	GLN
1	F	6030	HIS
1	F	6079	ASN
1	F	6095	GLN
1	F	6107	ASN
1	F	6131	ASN
1	F	6140	HIS
1	F	6162	ASN
1	F	6211	ASN
1	F	6241	HIS
1	F	6351	ASN
1	F	6353	GLN
1	F	6436	ASN
1	F	6532	ASN

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Mol	Chain	Res	Type
1	G	1045	GLN
1	G	1079	ASN
1	G	1107	ASN
1	G	1140	HIS
1	G	1169	GLN
1	G	1194	GLN
1	G	1211	ASN
1	G	1241	HIS
1	G	1267	GLN
1	G	1284	HIS
1	G	1288	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	H	2045	GLN
1	H	2069	GLN
1	H	2107	ASN
1	H	2140	HIS
1	H	2184	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	2532	ASN
1	H	2534	GLN
1	H	2537	GLN
1	I	3095	GLN
1	I	3140	HIS
1	I	3160	HIS
1	I	3184	HIS
1	I	3202	GLN
1	I	3211	ASN
1	I	3241	HIS
1	I	3267	GLN
1	I	3316	GLN
1	I	3336	GLN

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Mol	Chain	Res	Type
1	I	3342	HIS
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
1	J	4069	GLN
1	J	4079	ASN
1	J	4095	GLN
1	J	4107	ASN
1	J	4140	HIS
1	J	4184	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	4528	GLN
1	J	4532	ASN
1	J	4537	GLN
1	K	5045	GLN
1	K	5069	GLN
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	5351	ASN
1	K	5353	GLN
1	K	5436	ASN
1	K	5437	HIS
1	K	5450	GLN
1	K	5502	ASN
1	K	5522	GLN
1	K	5537	GLN

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Mol	Chain	Res	Type
1	L	6107	ASN
1	L	6140	HIS
1	L	6184	HIS
1	L	6238	ASN
1	L	6241	HIS
1	L	6309	GLN
1	L	6351	ASN
1	L	6353	GLN
1	L	6375	GLN
1	L	6450	GLN
1	L	6506	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
2	NAG	C	379	-	14,14,15	0.48	0	17,19,21	0.76	0
2	NAG	E	579	-	14,14,15	0.52	0	17,19,21	0.80	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NLX	K	5	-	26,29,29	3.23	14 (53%)	44,49,49	2.05	12 (27%)
3	NLX	G	1	-	26,29,29	3.47	15 (57%)	44,49,49	2.19	12 (27%)
2	NAG	J	479	-	14,14,15	0.56	0	17,19,21	0.67	0
3	NLX	A	1	-	26,29,29	3.76	15 (57%)	44,49,49	2.14	15 (34%)
3	NLX	L	6	-	26,29,29	3.42	16 (61%)	44,49,49	2.15	13 (29%)
3	NLX	D	4	-	26,29,29	3.37	16 (61%)	44,49,49	2.23	13 (29%)
2	NAG	K	579	-	14,14,15	0.53	0	17,19,21	0.78	1 (5%)
3	NLX	I	3	-	26,29,29	3.22	17 (65%)	44,49,49	2.33	14 (31%)
2	NAG	D	479	-	14,14,15	0.45	0	17,19,21	0.64	0
3	NLX	F	6	-	26,29,29	3.44	18 (69%)	44,49,49	4.85	23 (52%)
3	NLX	J	4	-	26,29,29	3.49	14 (53%)	44,49,49	1.98	12 (27%)
2	NAG	G	179	-	14,14,15	0.57	0	17,19,21	0.60	0
2	NAG	F	679	-	14,14,15	0.51	0	17,19,21	0.79	1 (5%)
2	NAG	I	379	-	14,14,15	0.47	0	17,19,21	0.82	1 (5%)
2	NAG	H	279	-	14,14,15	0.49	0	17,19,21	0.68	0
3	NLX	E	5	-	26,29,29	3.13	16 (61%)	44,49,49	2.01	13 (29%)
3	NLX	C	3	-	26,29,29	4.49	17 (65%)	44,49,49	4.63	18 (40%)
2	NAG	A	179	-	14,14,15	0.66	0	17,19,21	0.68	0
2	NAG	B	279	-	14,14,15	0.50	0	17,19,21	0.61	0
2	NAG	L	679	-	14,14,15	0.62	0	17,19,21	0.67	0
3	NLX	H	2	-	26,29,29	3.35	15 (57%)	44,49,49	2.41	12 (27%)
3	NLX	B	2	-	26,29,29	3.01	15 (57%)	44,49,49	2.03	11 (25%)
2	NAG	A	180	-	14,14,15	0.61	0	17,19,21	0.68	0

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
2	NAG	C	379	-	-	2/6/23/26	0/1/1/1
2	NAG	E	579	-	-	0/6/23/26	0/1/1/1
3	NLX	K	5	-	1/1/6/7	0/4/62/62	0/6/5/5
3	NLX	G	1	-	1/1/6/7	1/4/62/62	0/6/5/5
2	NAG	J	479	-	-	4/6/23/26	0/1/1/1
3	NLX	A	1	-	1/1/6/7	0/4/62/62	0/6/5/5
3	NLX	L	6	-	1/1/6/7	0/4/62/62	0/6/5/5
3	NLX	D	4	-	1/1/6/7	0/4/62/62	0/6/5/5
2	NAG	K	579	-	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NLX	I	3	-	1/1/6/7	1/4/62/62	0/6/5/5
2	NAG	D	479	-	-	2/6/23/26	0/1/1/1
3	NLX	F	6	-	1/1/6/7	2/4/62/62	0/6/5/5
3	NLX	J	4	-	1/1/6/7	0/4/62/62	0/6/5/5
2	NAG	G	179	-	-	5/6/23/26	0/1/1/1
2	NAG	F	679	-	-	3/6/23/26	0/1/1/1
2	NAG	I	379	-	-	4/6/23/26	0/1/1/1
2	NAG	H	279	-	-	4/6/23/26	0/1/1/1
3	NLX	E	5	-	1/1/6/7	0/4/62/62	0/6/5/5
3	NLX	C	3	-	1/1/6/7	1/4/62/62	0/6/5/5
2	NAG	A	179	-	-	4/6/23/26	0/1/1/1
2	NAG	B	279	-	-	2/6/23/26	0/1/1/1
2	NAG	L	679	-	-	2/6/23/26	0/1/1/1
3	NLX	H	2	-	1/1/6/7	0/4/62/62	0/6/5/5
3	NLX	B	2	-	1/1/6/7	0/4/62/62	0/6/5/5
2	NAG	A	180	-	-	2/6/23/26	0/1/1/1

All (188) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	3	NLX	C14-C9	15.46	1.78	1.55
3	D	4	NLX	C14-C9	10.69	1.71	1.55
3	H	2	NLX	C14-C9	10.43	1.71	1.55
3	J	4	NLX	C14-C9	10.06	1.70	1.55
3	A	1	NLX	C14-C9	9.94	1.70	1.55
3	I	3	NLX	C14-C9	9.05	1.69	1.55
3	L	6	NLX	C14-C9	8.81	1.68	1.55
3	G	1	NLX	C14-C9	8.66	1.68	1.55
3	K	5	NLX	C14-C9	8.41	1.68	1.55
3	E	5	NLX	C14-C9	8.29	1.67	1.55
3	A	1	NLX	C14-C13	7.46	1.63	1.53
3	F	6	NLX	C11-C12	7.18	1.50	1.39
3	F	6	NLX	C14-C13	7.08	1.63	1.53
3	L	6	NLX	C14-C13	7.03	1.63	1.53
3	G	1	NLX	C14-C13	6.87	1.62	1.53
3	I	3	NLX	C14-C13	6.65	1.62	1.53
3	K	5	NLX	C14-C13	6.64	1.62	1.53
3	B	2	NLX	C14-C9	6.60	1.65	1.55
3	B	2	NLX	C14-C13	6.54	1.62	1.53
3	C	3	NLX	C14-C13	6.49	1.62	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	2	NLX	C14-C13	6.49	1.62	1.53
3	J	4	NLX	C14-C13	6.42	1.62	1.53
3	E	5	NLX	C14-C13	6.13	1.61	1.53
3	A	1	NLX	C15-C13	5.85	1.62	1.54
3	D	4	NLX	C14-C13	5.80	1.61	1.53
3	C	3	NLX	C10-C11	5.55	1.62	1.51
3	L	6	NLX	C15-C13	5.49	1.61	1.54
3	C	3	NLX	C11-C12	5.49	1.48	1.39
3	F	6	NLX	C14-C9	5.46	1.63	1.55
3	G	1	NLX	C8-C14	5.41	1.60	1.53
3	G	1	NLX	C15-C13	5.33	1.61	1.54
3	C	3	NLX	C13-C5	5.28	1.61	1.54
3	A	1	NLX	C8-C14	5.23	1.60	1.53
3	C	3	NLX	C8-C14	5.13	1.60	1.53
3	J	4	NLX	C8-C14	4.89	1.60	1.53
3	I	3	NLX	C15-C13	4.87	1.60	1.54
3	B	2	NLX	C15-C13	4.85	1.60	1.54
3	A	1	NLX	C16-C15	4.82	1.60	1.52
3	J	4	NLX	C13-C5	4.77	1.60	1.54
3	A	1	NLX	C13-C5	4.75	1.60	1.54
3	K	5	NLX	C15-C13	4.71	1.60	1.54
3	H	2	NLX	C15-C13	4.67	1.60	1.54
3	J	4	NLX	C15-C13	4.58	1.60	1.54
3	E	5	NLX	C15-C13	4.58	1.60	1.54
3	D	4	NLX	C15-C13	4.53	1.60	1.54
3	L	6	NLX	C8-C14	4.51	1.59	1.53
3	D	4	NLX	C11-C12	4.50	1.46	1.39
3	C	3	NLX	O2-C5	4.49	1.54	1.46
3	F	6	NLX	C16-C15	4.48	1.60	1.52
3	F	6	NLX	C8-C7	4.39	1.62	1.53
3	B	2	NLX	C11-C12	4.24	1.46	1.39
3	G	1	NLX	C16-C15	4.09	1.59	1.52
3	K	5	NLX	C10-C11	4.05	1.59	1.51
3	D	4	NLX	C8-C14	4.04	1.58	1.53
3	L	6	NLX	C10-C11	4.04	1.59	1.51
3	J	4	NLX	C11-C12	4.04	1.45	1.39
3	E	5	NLX	C10-C11	4.04	1.59	1.51
3	G	1	NLX	C13-C5	4.02	1.59	1.54
3	F	6	NLX	C17-C18	3.99	1.63	1.49
3	A	1	NLX	C7-C6	3.99	1.57	1.50
3	H	2	NLX	C8-C14	3.99	1.58	1.53
3	J	4	NLX	C16-C15	3.99	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	2	NLX	C11-C12	3.93	1.45	1.39
3	K	5	NLX	C8-C14	3.92	1.58	1.53
3	L	6	NLX	C16-C15	3.92	1.59	1.52
3	G	1	NLX	C10-C11	3.88	1.58	1.51
3	F	6	NLX	C2-C3	3.87	1.46	1.39
3	I	3	NLX	C11-C12	3.84	1.45	1.39
3	F	6	NLX	O2-C5	3.84	1.53	1.46
3	G	1	NLX	C11-C12	3.84	1.45	1.39
3	A	1	NLX	C11-C12	3.79	1.45	1.39
3	K	5	NLX	C7-C6	3.78	1.57	1.50
3	H	2	NLX	C13-C5	3.78	1.59	1.54
3	C	3	NLX	C4-C12	3.78	1.43	1.38
3	J	4	NLX	C7-C6	3.75	1.57	1.50
3	G	1	NLX	C7-C6	3.74	1.57	1.50
3	L	6	NLX	C7-C6	3.68	1.56	1.50
3	K	5	NLX	C11-C12	3.66	1.45	1.39
3	B	2	NLX	C16-C15	3.65	1.58	1.52
3	F	6	NLX	C20-N1	3.60	1.61	1.50
3	K	5	NLX	C16-C15	3.59	1.58	1.52
3	F	6	NLX	C7-C6	3.57	1.56	1.50
3	B	2	NLX	C8-C14	3.57	1.58	1.53
3	D	4	NLX	C10-C11	3.55	1.58	1.51
3	E	5	NLX	C16-C15	3.54	1.58	1.52
3	A	1	NLX	C10-C11	3.53	1.58	1.51
3	I	3	NLX	C13-C5	3.50	1.59	1.54
3	K	5	NLX	C2-C1	3.47	1.44	1.38
3	F	6	NLX	C13-C5	3.46	1.59	1.54
3	L	6	NLX	C13-C5	3.43	1.59	1.54
3	C	3	NLX	C8-C7	3.40	1.60	1.53
3	D	4	NLX	C13-C5	3.35	1.58	1.54
3	I	3	NLX	C16-C15	3.34	1.58	1.52
3	A	1	NLX	C4-C12	3.33	1.43	1.38
3	H	2	NLX	C7-C6	3.28	1.56	1.50
3	B	2	NLX	C10-C11	3.28	1.57	1.51
3	C	3	NLX	C13-C12	3.25	1.56	1.50
3	D	4	NLX	C7-C6	3.24	1.56	1.50
3	E	5	NLX	C8-C14	3.23	1.57	1.53
3	L	6	NLX	C4-C12	3.19	1.42	1.38
3	C	3	NLX	C7-C6	3.17	1.56	1.50
3	J	4	NLX	C4-C12	3.17	1.42	1.38
3	C	3	NLX	C3-C4	3.13	1.46	1.40
3	F	6	NLX	C8-C14	3.13	1.57	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	5	NLX	C11-C12	3.09	1.44	1.39
3	I	3	NLX	C8-C14	3.08	1.57	1.53
3	G	1	NLX	C5-C6	3.07	1.60	1.52
3	E	5	NLX	C2-C1	3.05	1.43	1.38
3	B	2	NLX	C2-C1	3.04	1.43	1.38
3	F	6	NLX	C13-C12	3.03	1.56	1.50
3	B	2	NLX	C13-C5	3.02	1.58	1.54
3	L	6	NLX	C11-C12	3.02	1.44	1.39
3	H	2	NLX	C8-C7	3.00	1.59	1.53
3	E	5	NLX	C13-C5	3.00	1.58	1.54
3	G	1	NLX	C2-C1	3.00	1.43	1.38
3	C	3	NLX	C2-C1	2.99	1.43	1.38
3	K	5	NLX	C4-C12	2.98	1.42	1.38
3	E	5	NLX	C7-C6	2.97	1.55	1.50
3	J	4	NLX	C8-C7	2.97	1.59	1.53
3	L	6	NLX	C2-C1	2.93	1.43	1.38
3	A	1	NLX	C2-C1	2.92	1.43	1.38
3	E	5	NLX	C4-C12	2.91	1.42	1.38
3	I	3	NLX	C7-C6	2.90	1.55	1.50
3	E	5	NLX	O2-C5	2.87	1.51	1.46
3	L	6	NLX	C5-C6	2.87	1.59	1.52
3	H	2	NLX	C16-C15	2.86	1.57	1.52
3	B	2	NLX	O2-C5	2.86	1.51	1.46
3	I	3	NLX	C13-C12	2.85	1.56	1.50
3	G	1	NLX	C4-C12	2.84	1.42	1.38
3	E	5	NLX	C5-C6	2.84	1.59	1.52
3	J	4	NLX	C10-C11	2.82	1.56	1.51
3	D	4	NLX	C16-C15	2.79	1.57	1.52
3	H	2	NLX	O2-C5	2.79	1.51	1.46
3	K	5	NLX	C13-C5	2.79	1.58	1.54
3	I	3	NLX	C3-C4	2.75	1.45	1.40
3	L	6	NLX	O2-C5	2.75	1.51	1.46
3	B	2	NLX	C5-C6	2.73	1.59	1.52
3	D	4	NLX	C8-C7	2.72	1.58	1.53
3	I	3	NLX	C5-C6	2.72	1.59	1.52
3	C	3	NLX	C15-C13	2.69	1.57	1.54
3	B	2	NLX	C4-C12	2.68	1.42	1.38
3	D	4	NLX	C2-C1	2.65	1.43	1.38
3	D	4	NLX	C4-C12	2.63	1.42	1.38
3	H	2	NLX	C10-C11	2.62	1.56	1.51
3	C	3	NLX	O2-C4	2.61	1.42	1.38
3	A	1	NLX	C8-C7	2.57	1.58	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	4	NLX	C2-C1	2.55	1.42	1.38
3	B	2	NLX	C13-C12	2.55	1.55	1.50
3	A	1	NLX	C5-C6	2.54	1.59	1.52
3	B	2	NLX	C2-C3	2.48	1.43	1.39
3	K	5	NLX	C5-C6	2.45	1.58	1.52
3	C	3	NLX	C16-C15	2.45	1.56	1.52
3	E	5	NLX	C3-C4	2.45	1.45	1.40
3	G	1	NLX	O2-C5	2.42	1.50	1.46
3	I	3	NLX	C2-C1	2.42	1.42	1.38
3	I	3	NLX	C10-C11	2.42	1.56	1.51
3	I	3	NLX	C4-C12	2.39	1.41	1.38
3	B	2	NLX	C7-C6	2.39	1.54	1.50
3	L	6	NLX	C3-C4	2.37	1.45	1.40
3	F	6	NLX	C16-N1	2.37	1.57	1.52
3	C	3	NLX	C2-C3	2.34	1.43	1.39
3	H	2	NLX	C3-C4	2.34	1.45	1.40
3	A	1	NLX	O2-C5	2.31	1.50	1.46
3	G	1	NLX	C8-C7	2.29	1.57	1.53
3	I	3	NLX	O2-C5	2.28	1.50	1.46
3	F	6	NLX	C19-C18	2.26	1.43	1.29
3	J	4	NLX	O2-C5	2.25	1.50	1.46
3	F	6	NLX	C10-C11	2.23	1.55	1.51
3	H	2	NLX	C4-C12	2.23	1.41	1.38
3	I	3	NLX	C2-C3	2.21	1.43	1.39
3	K	5	NLX	C1-C11	2.19	1.43	1.39
3	G	1	NLX	C2-C3	2.18	1.43	1.39
3	K	5	NLX	C2-C3	2.17	1.43	1.39
3	D	4	NLX	O2-C5	2.17	1.50	1.46
3	D	4	NLX	C5-C6	2.12	1.58	1.52
3	A	1	NLX	C3-C4	2.11	1.44	1.40
3	H	2	NLX	C13-C12	2.10	1.54	1.50
3	D	4	NLX	C2-C3	2.09	1.43	1.39
3	L	6	NLX	C13-C12	2.08	1.54	1.50
3	D	4	NLX	C3-C4	2.08	1.44	1.40
3	E	5	NLX	C1-C11	2.08	1.43	1.39
3	F	6	NLX	C5-C6	2.07	1.57	1.52
3	I	3	NLX	C8-C7	2.07	1.57	1.53
3	L	6	NLX	C1-C11	2.05	1.43	1.39
3	E	5	NLX	C8-C7	2.05	1.57	1.53
3	F	6	NLX	O3-C6	2.01	1.25	1.21
3	H	2	NLX	C5-C6	2.01	1.57	1.52
3	J	4	NLX	C5-C6	2.00	1.57	1.52

All (172) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	3	NLX	C20-N1-C17	-19.90	63.74	107.94
3	F	6	NLX	C20-N1-C17	-18.82	66.14	107.94
3	C	3	NLX	C20-N1-C16	-15.60	68.71	108.71
3	F	6	NLX	C20-N1-C16	-14.40	71.79	108.71
3	F	6	NLX	O2-C5-C6	10.12	116.90	108.51
3	F	6	NLX	C15-C13-C14	8.93	116.41	109.38
3	C	3	NLX	C16-N1-C17	8.82	131.74	109.30
3	F	6	NLX	C16-N1-C17	8.04	129.74	109.30
3	G	1	NLX	O2-C5-C6	7.76	114.94	108.51
3	H	2	NLX	C18-C17-N1	7.68	124.99	114.34
3	I	3	NLX	O2-C5-C6	7.46	114.70	108.51
3	I	3	NLX	C18-C17-N1	7.20	124.33	114.34
3	B	2	NLX	O2-C5-C6	6.73	114.09	108.51
3	K	5	NLX	O2-C5-C6	6.51	113.91	108.51
3	L	6	NLX	O2-C5-C6	6.50	113.90	108.51
3	D	4	NLX	C18-C17-N1	6.50	123.35	114.34
3	F	6	NLX	C13-C14-C9	6.12	110.30	106.34
3	F	6	NLX	C14-C13-C5	6.04	122.62	118.08
3	E	5	NLX	O2-C5-C6	5.88	113.38	108.51
3	H	2	NLX	O2-C5-C6	5.88	113.38	108.51
3	B	2	NLX	C18-C17-N1	5.71	122.26	114.34
3	J	4	NLX	C18-C17-N1	5.68	122.22	114.34
3	A	1	NLX	C18-C17-N1	5.44	121.89	114.34
3	L	6	NLX	C18-C17-N1	5.27	121.66	114.34
3	C	3	NLX	C10-C9-C14	-5.22	104.30	114.66
3	C	3	NLX	O2-C5-C6	5.17	112.80	108.51
3	G	1	NLX	C18-C17-N1	5.17	121.51	114.34
3	A	1	NLX	O2-C5-C6	5.11	112.74	108.51
3	D	4	NLX	O2-C5-C6	4.96	112.62	108.51
3	H	2	NLX	C8-C14-C13	-4.95	107.38	111.52
3	C	3	NLX	C8-C14-C13	-4.90	107.42	111.52
3	K	5	NLX	C18-C17-N1	4.76	120.94	114.34
3	D	4	NLX	C8-C14-C9	4.51	118.06	111.71
3	H	2	NLX	C8-C14-C9	4.43	117.95	111.71
3	L	6	NLX	C7-C6-C5	4.40	123.33	116.45
3	G	1	NLX	C7-C6-C5	4.31	123.21	116.45
3	D	4	NLX	C8-C14-C13	-4.27	107.95	111.52
3	K	5	NLX	C7-C6-C5	4.20	123.03	116.45
3	E	5	NLX	C7-C6-C5	4.16	122.97	116.45
3	A	1	NLX	C8-C14-C9	4.12	117.51	111.71
3	C	3	NLX	C8-C14-C9	4.11	117.50	111.71
3	A	1	NLX	C7-C6-C5	4.09	122.85	116.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2	NLX	C7-C6-C5	4.07	122.82	116.45
3	D	4	NLX	C17-N1-C9	4.06	117.77	110.24
3	J	4	NLX	C8-C14-C9	4.04	117.40	111.71
3	J	4	NLX	C8-C14-C13	-4.03	108.15	111.52
3	H	2	NLX	C17-N1-C9	3.94	117.56	110.24
3	F	6	NLX	C15-C13-C12	-3.90	103.26	111.50
3	F	6	NLX	C8-C14-C9	3.90	117.20	111.71
3	J	4	NLX	C7-C6-C5	3.88	122.53	116.45
3	A	1	NLX	C8-C14-C13	-3.86	108.29	111.52
3	I	3	NLX	C8-C14-C13	-3.86	108.30	111.52
3	G	1	NLX	C10-C9-C14	-3.83	107.06	114.66
3	I	3	NLX	C7-C6-C5	3.78	122.37	116.45
3	C	3	NLX	C16-N1-C9	-3.77	98.54	109.17
3	D	4	NLX	C7-C6-C5	3.76	122.34	116.45
3	E	5	NLX	C18-C17-N1	3.74	119.53	114.34
3	C	3	NLX	C13-C12-C4	3.67	112.57	109.23
3	E	5	NLX	C8-C14-C9	3.65	116.85	111.71
3	A	1	NLX	C10-C9-C14	-3.64	107.44	114.66
3	H	2	NLX	C7-C6-C5	3.63	122.14	116.45
3	G	1	NLX	C8-C14-C9	3.60	116.78	111.71
3	C	3	NLX	O2-C4-C3	3.56	132.36	126.14
3	L	6	NLX	C8-C14-C9	3.53	116.68	111.71
3	E	5	NLX	C10-C9-C14	-3.53	107.66	114.66
3	J	4	NLX	O2-C5-C6	3.53	111.43	108.51
3	K	5	NLX	C10-C9-C14	-3.50	107.72	114.66
3	K	5	NLX	C8-C14-C9	3.46	116.59	111.71
3	F	6	NLX	C14-C13-C12	-3.38	104.02	108.48
3	L	6	NLX	C10-C9-C14	-3.38	107.95	114.66
3	E	5	NLX	C8-C14-C13	-3.37	108.70	111.52
3	A	1	NLX	C13-C12-C4	3.27	112.21	109.23
3	I	3	NLX	C8-C14-C9	3.27	116.32	111.71
3	F	6	NLX	O2-C4-C3	3.27	131.85	126.14
3	F	6	NLX	C13-C12-C4	3.23	112.17	109.23
3	B	2	NLX	O3-C6-C7	-3.23	116.38	122.13
3	L	6	NLX	C13-C12-C4	3.21	112.16	109.23
3	K	5	NLX	C15-C13-C14	3.20	111.90	109.38
3	J	4	NLX	C10-C9-C14	-3.18	108.35	114.66
3	H	2	NLX	O2-C4-C3	3.16	131.66	126.14
3	B	2	NLX	C10-C9-C14	-3.11	108.49	114.66
3	C	3	NLX	C7-C6-C5	3.08	121.27	116.45
3	H	2	NLX	C13-C12-C4	3.06	112.02	109.23
3	F	6	NLX	C12-C13-C5	-3.06	95.56	98.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	6	NLX	O2-C4-C12	-3.03	109.30	112.80
3	F	6	NLX	C17-N1-C9	-3.00	104.68	110.24
3	L	6	NLX	C8-C14-C13	-2.96	109.04	111.52
3	E	5	NLX	O2-C4-C3	2.96	131.31	126.14
3	E	5	NLX	C13-C12-C4	2.95	111.92	109.23
3	I	3	NLX	O2-C4-C3	2.94	131.28	126.14
3	D	4	NLX	C10-C9-C14	-2.93	108.84	114.66
3	C	3	NLX	O2-C4-C12	-2.91	109.44	112.80
3	I	3	NLX	C13-C12-C4	2.91	111.88	109.23
3	E	5	NLX	O2-C4-C12	-2.89	109.45	112.80
3	L	6	NLX	O2-C4-C3	2.89	131.19	126.14
3	C	3	NLX	C13-C14-C9	2.87	108.20	106.34
3	A	1	NLX	O2-C4-C3	2.87	131.15	126.14
3	F	6	NLX	C8-C14-C13	-2.86	109.13	111.52
3	C	3	NLX	C14-C13-C5	2.85	120.22	118.08
3	G	1	NLX	O2-C4-C3	2.85	131.11	126.14
3	H	2	NLX	C10-C9-C14	-2.84	109.02	114.66
3	D	4	NLX	O2-C4-C3	2.84	131.10	126.14
3	E	5	NLX	O3-C6-C7	-2.83	117.09	122.13
3	B	2	NLX	O2-C4-C3	2.82	131.06	126.14
3	F	6	NLX	C7-C6-C5	2.78	120.81	116.45
3	G	1	NLX	C15-C13-C14	2.78	111.57	109.38
3	I	3	NLX	O2-C4-C12	-2.77	109.60	112.80
3	D	4	NLX	C15-C13-C14	2.75	111.54	109.38
3	A	1	NLX	C20-N1-C17	-2.74	101.85	107.94
3	F	6	NLX	O4-C14-C8	-2.74	102.28	107.97
3	J	4	NLX	C13-C12-C4	2.73	111.72	109.23
3	J	4	NLX	O2-C4-C3	2.73	130.91	126.14
3	C	3	NLX	C15-C13-C14	-2.73	107.24	109.38
3	C	3	NLX	C15-C13-C5	2.70	114.87	111.97
3	L	6	NLX	C15-C13-C14	2.69	111.50	109.38
3	B	2	NLX	C8-C14-C13	-2.69	109.28	111.52
3	G	1	NLX	O3-C6-C7	-2.68	117.35	122.13
3	F	6	NLX	C3-C4-C12	-2.68	117.71	120.97
3	K	5	NLX	C8-C14-C13	-2.67	109.28	111.52
3	K	5	NLX	O2-C4-C12	-2.64	109.75	112.80
3	G	1	NLX	C13-C12-C4	2.64	111.63	109.23
3	I	3	NLX	O3-C6-C7	-2.61	117.47	122.13
3	L	6	NLX	O3-C6-C7	-2.61	117.48	122.13
3	K	5	NLX	O2-C4-C3	2.60	130.68	126.14
3	H	2	NLX	O2-C4-C12	-2.60	109.80	112.80
3	I	3	NLX	C10-C9-C14	-2.59	109.52	114.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	3	NLX	C17-N1-C9	-2.58	105.45	110.24
3	B	2	NLX	C13-C12-C4	2.57	111.57	109.23
3	K	5	NLX	C13-C12-C4	2.57	111.57	109.23
3	B	2	NLX	O2-C4-C12	-2.54	109.86	112.80
3	A	1	NLX	O2-C4-C12	-2.54	109.86	112.80
3	H	2	NLX	C14-C13-C5	2.53	119.98	118.08
3	D	4	NLX	O2-C4-C12	-2.53	109.88	112.80
3	L	6	NLX	C20-N1-C17	-2.50	102.39	107.94
3	A	1	NLX	C12-C13-C5	-2.50	96.09	98.46
3	I	3	NLX	C12-C13-C5	-2.49	96.10	98.46
2	I	379	NAG	C2-N2-C7	-2.44	119.63	122.90
3	G	1	NLX	O2-C4-C12	-2.44	109.98	112.80
3	D	4	NLX	C13-C12-C4	2.43	111.44	109.23
3	G	1	NLX	C15-C13-C12	-2.41	106.40	111.50
3	A	1	NLX	C15-C13-C14	2.39	111.26	109.38
3	K	5	NLX	O3-C6-C7	-2.38	117.89	122.13
3	J	4	NLX	C20-N1-C17	-2.37	102.67	107.94
3	G	1	NLX	C8-C14-C13	-2.37	109.54	111.52
3	E	5	NLX	C15-C13-C14	2.36	111.24	109.38
2	K	579	NAG	C2-N2-C7	-2.36	119.74	122.90
3	E	5	NLX	C17-N1-C9	2.36	114.62	110.24
3	H	2	NLX	C15-C13-C14	2.36	111.24	109.38
3	L	6	NLX	C12-C13-C5	-2.34	96.24	98.46
2	F	679	NAG	C2-N2-C7	-2.33	119.78	122.90
2	E	579	NAG	C2-N2-C7	-2.31	119.80	122.90
3	A	1	NLX	O3-C6-C7	-2.31	118.02	122.13
3	C	3	NLX	C3-C4-C12	-2.30	118.17	120.97
3	B	2	NLX	C12-C13-C5	-2.29	96.29	98.46
3	D	4	NLX	C4-O2-C5	2.27	107.29	104.83
3	I	3	NLX	C15-C13-C14	2.26	111.16	109.38
3	K	5	NLX	C12-C13-C5	-2.21	96.36	98.46
3	F	6	NLX	O4-C14-C9	-2.19	104.00	108.23
3	B	2	NLX	C15-C13-C14	2.11	111.04	109.38
3	F	6	NLX	C10-C9-C14	-2.10	110.48	114.66
3	A	1	NLX	C17-N1-C9	2.10	114.14	110.24
3	F	6	NLX	C16-N1-C9	2.09	115.06	109.17
3	A	1	NLX	O2-C5-C13	2.09	106.20	104.88
3	D	4	NLX	O3-C6-C7	-2.09	118.41	122.13
3	I	3	NLX	C17-N1-C9	2.08	114.10	110.24
3	J	4	NLX	O2-C5-C13	2.07	106.19	104.88
3	J	4	NLX	C17-N1-C9	2.07	114.08	110.24
3	F	6	NLX	O4-C14-C13	2.06	113.77	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	5	NLX	C20-N1-C17	-2.06	103.36	107.94
3	F	6	NLX	O2-C4-C12	-2.05	110.43	112.80
3	J	4	NLX	O2-C4-C12	-2.02	110.46	112.80
3	I	3	NLX	C13-C14-C9	-2.01	105.05	106.34

All (12) chirality outliers are listed below:

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

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	179	NAG	C8-C7-N2-C2
2	A	179	NAG	O7-C7-N2-C2
2	A	180	NAG	C8-C7-N2-C2
2	A	180	NAG	O7-C7-N2-C2
2	B	279	NAG	C8-C7-N2-C2
2	B	279	NAG	O7-C7-N2-C2
2	F	679	NAG	C8-C7-N2-C2
2	F	679	NAG	O7-C7-N2-C2
2	G	179	NAG	C1-C2-N2-C7
2	H	279	NAG	C8-C7-N2-C2
2	H	279	NAG	O7-C7-N2-C2
2	I	379	NAG	O7-C7-N2-C2
2	K	579	NAG	C8-C7-N2-C2
2	K	579	NAG	O7-C7-N2-C2
3	C	3	NLX	N1-C17-C18-C19
3	G	1	NLX	N1-C17-C18-C19
2	C	379	NAG	C8-C7-N2-C2
2	C	379	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
2	G	179	NAG	C8-C7-N2-C2
2	G	179	NAG	O7-C7-N2-C2
2	I	379	NAG	C8-C7-N2-C2
2	L	679	NAG	C8-C7-N2-C2
2	L	679	NAG	O7-C7-N2-C2
2	A	179	NAG	C4-C5-C6-O6
2	K	579	NAG	C4-C5-C6-O6
2	H	279	NAG	C4-C5-C6-O6
2	H	279	NAG	O5-C5-C6-O6
2	A	179	NAG	O5-C5-C6-O6
2	D	479	NAG	C8-C7-N2-C2
2	K	579	NAG	O5-C5-C6-O6
2	I	379	NAG	C4-C5-C6-O6
2	I	379	NAG	O5-C5-C6-O6
2	G	179	NAG	C4-C5-C6-O6
2	D	479	NAG	O7-C7-N2-C2
2	J	479	NAG	C3-C2-N2-C7
2	G	179	NAG	O5-C5-C6-O6
2	J	479	NAG	C1-C2-N2-C7
3	F	6	NLX	C18-C17-N1-C20
3	F	6	NLX	N1-C17-C18-C19
2	J	479	NAG	C8-C7-N2-C2
2	J	479	NAG	O7-C7-N2-C2
2	F	679	NAG	C4-C5-C6-O6
3	I	3	NLX	N1-C17-C18-C19

There are no ring outliers.

22 monomers are involved in 277 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	579	NAG	2	0
3	K	5	NLX	18	0
3	G	1	NLX	12	0
2	J	479	NAG	7	0
3	A	1	NLX	21	0
3	L	6	NLX	23	0
3	D	4	NLX	15	0
2	K	579	NAG	1	0
3	I	3	NLX	19	0
2	D	479	NAG	4	0
3	F	6	NLX	23	0
3	J	4	NLX	20	0

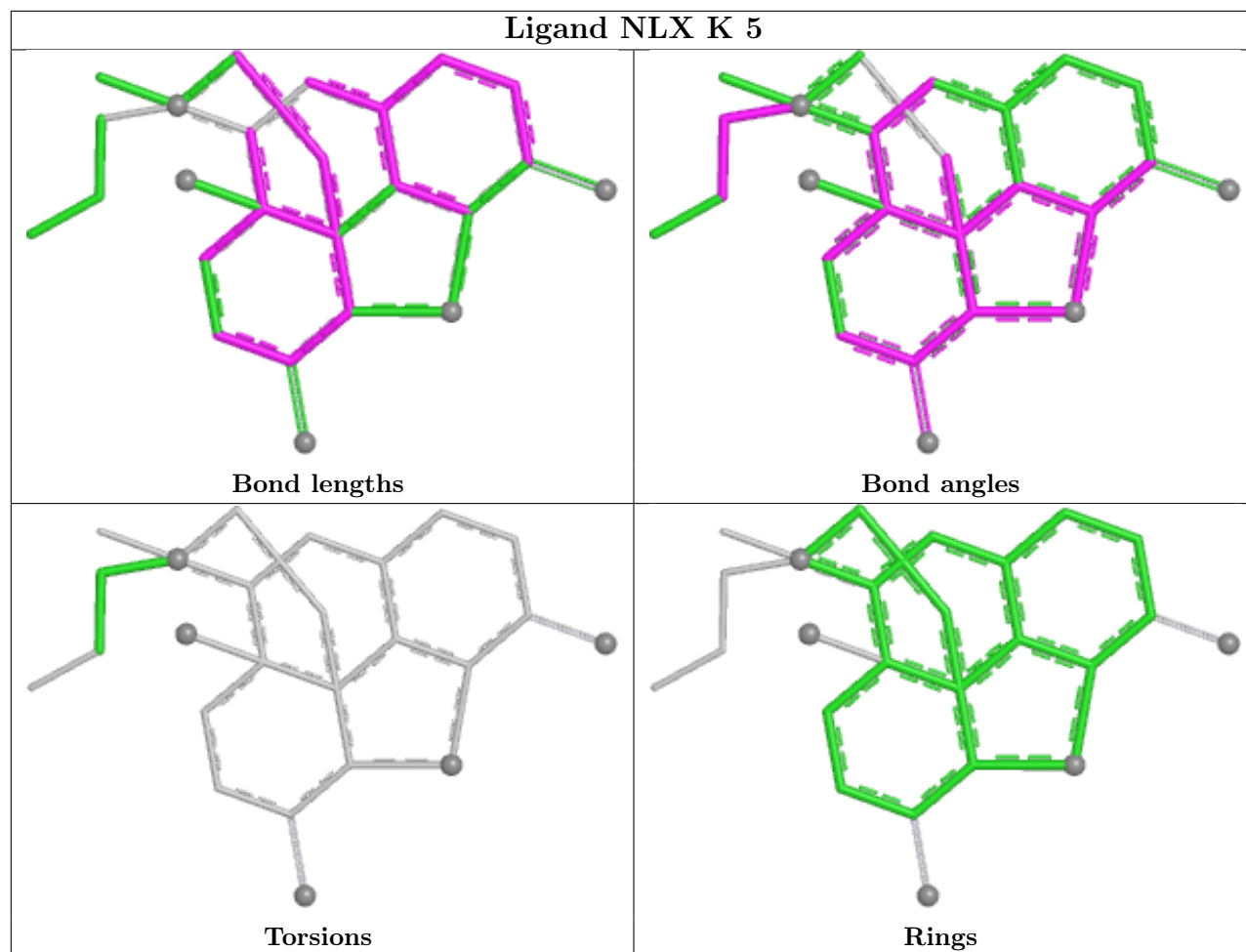
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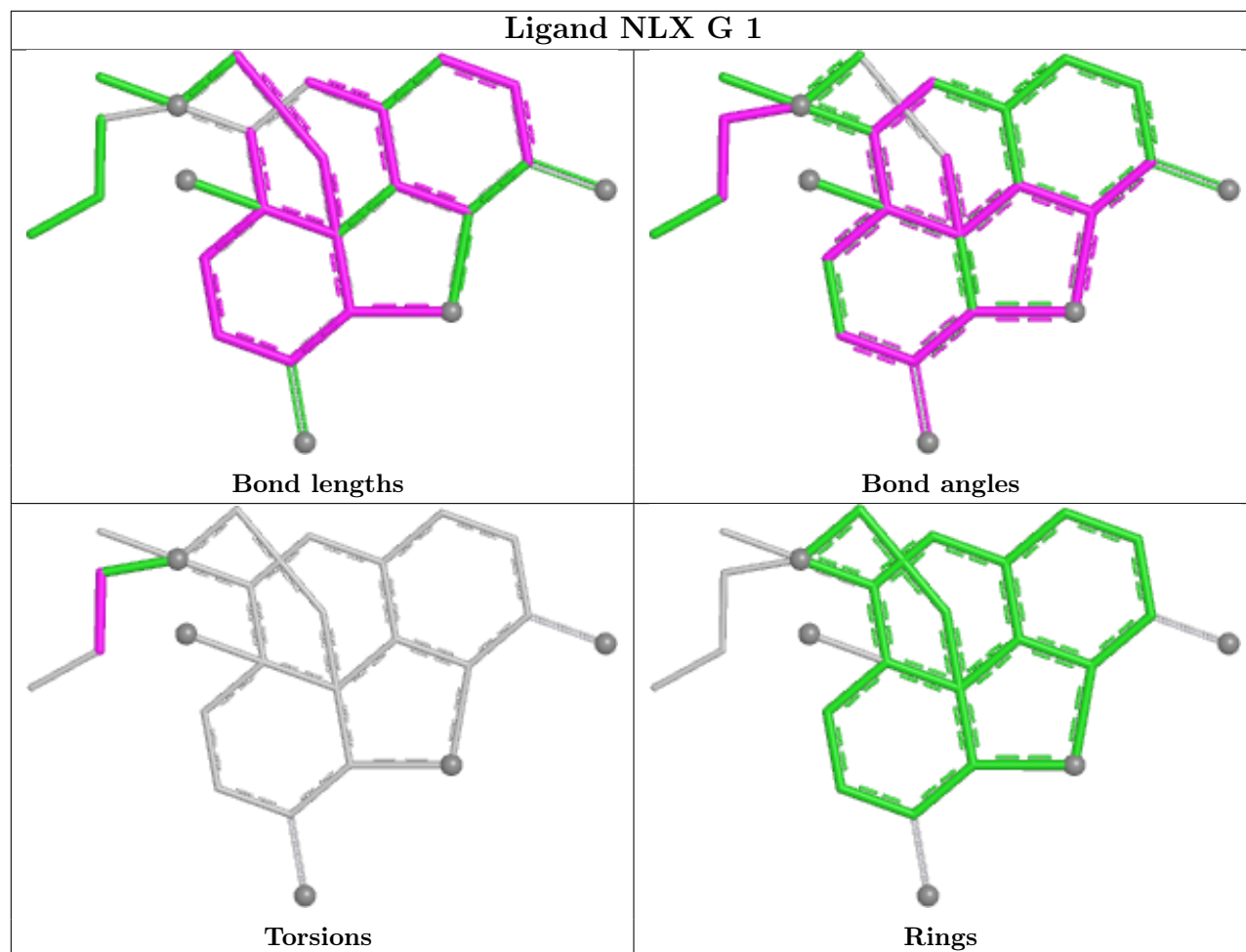
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	179	NAG	4	0
2	I	379	NAG	1	0
2	H	279	NAG	1	0
3	E	5	NLX	18	0
3	C	3	NLX	28	0
2	A	179	NAG	3	0
2	B	279	NAG	5	0
3	H	2	NLX	31	0
3	B	2	NLX	21	0
2	A	180	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

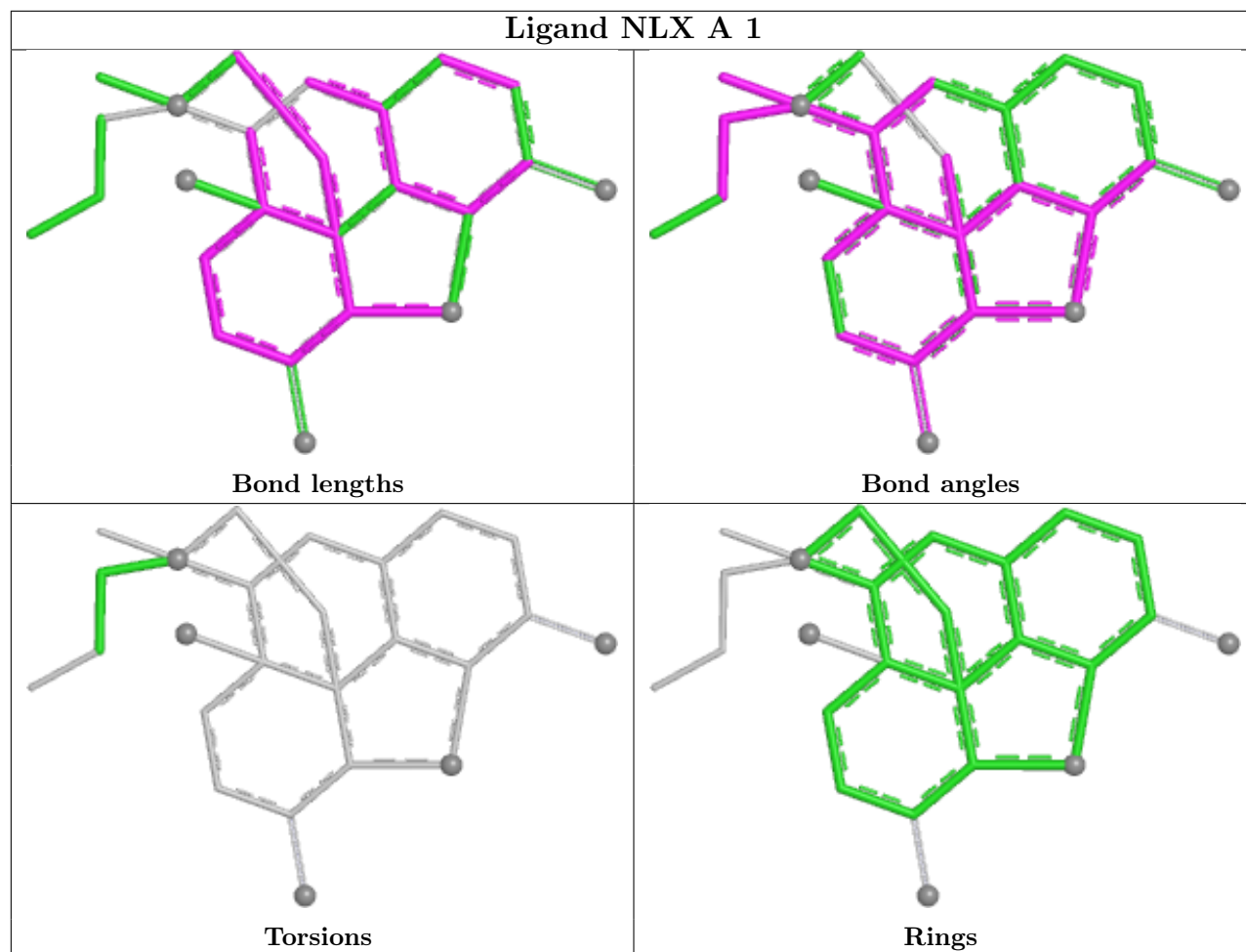
Ligand NLX K 5



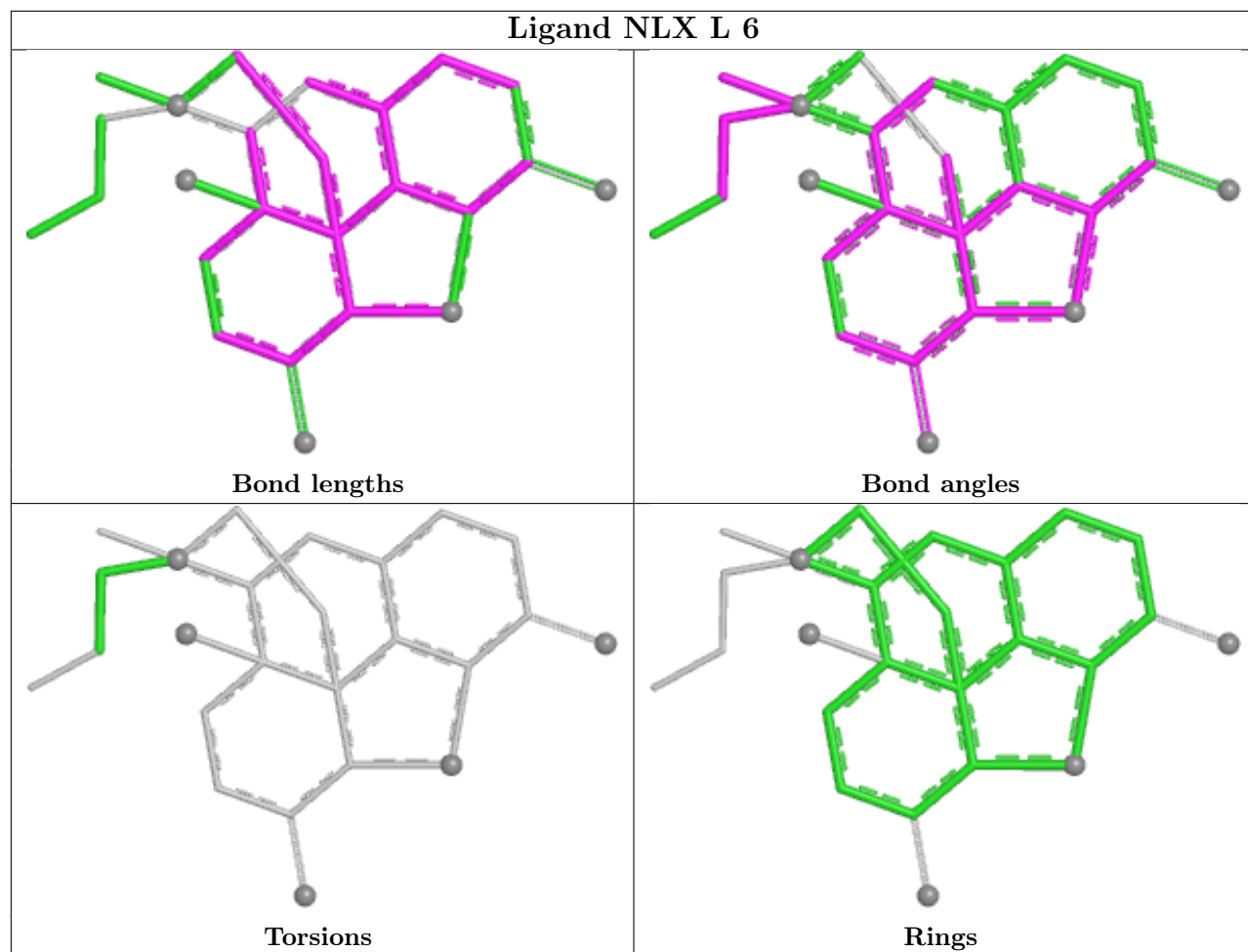
Ligand NLX G 1



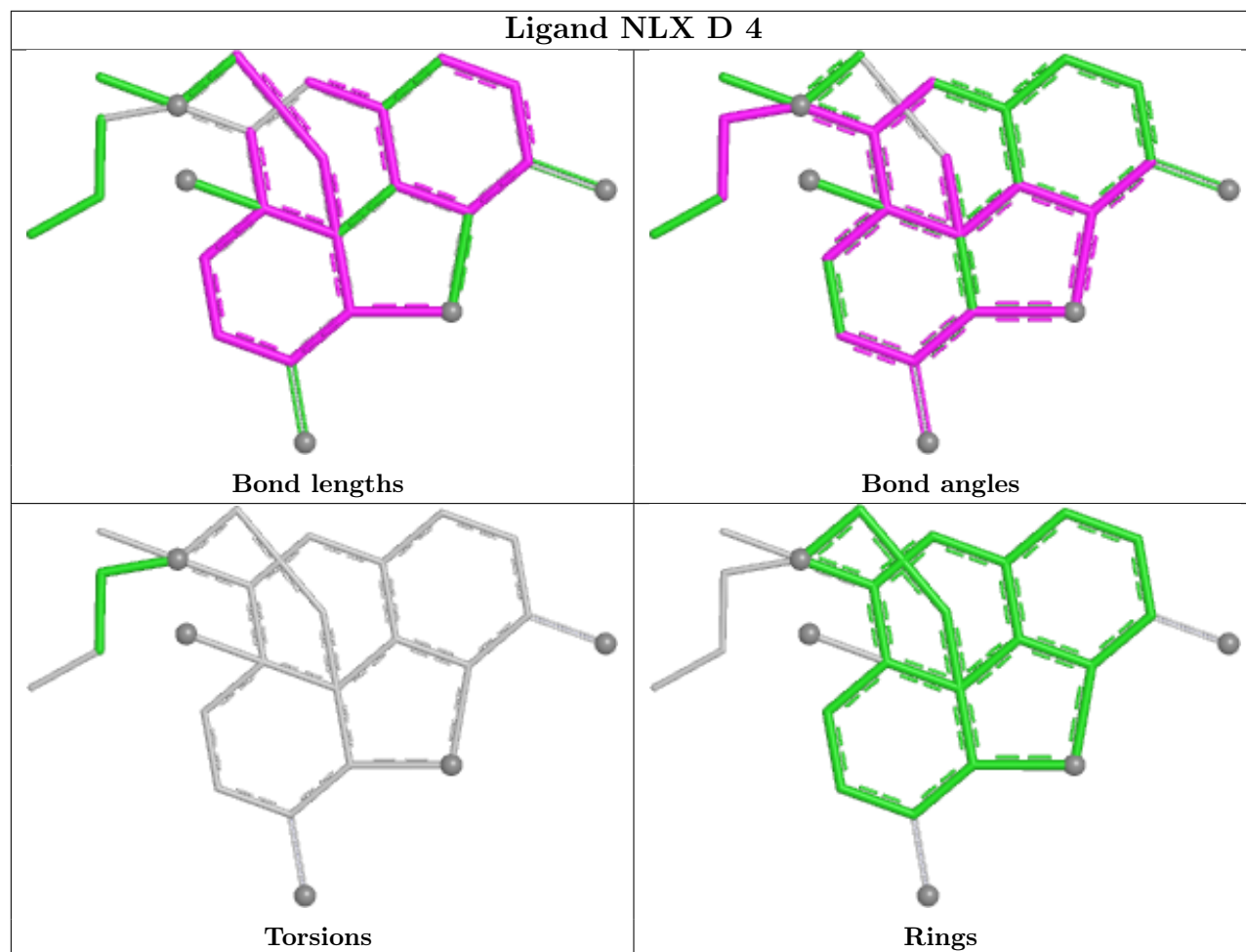
Ligand NLX A 1

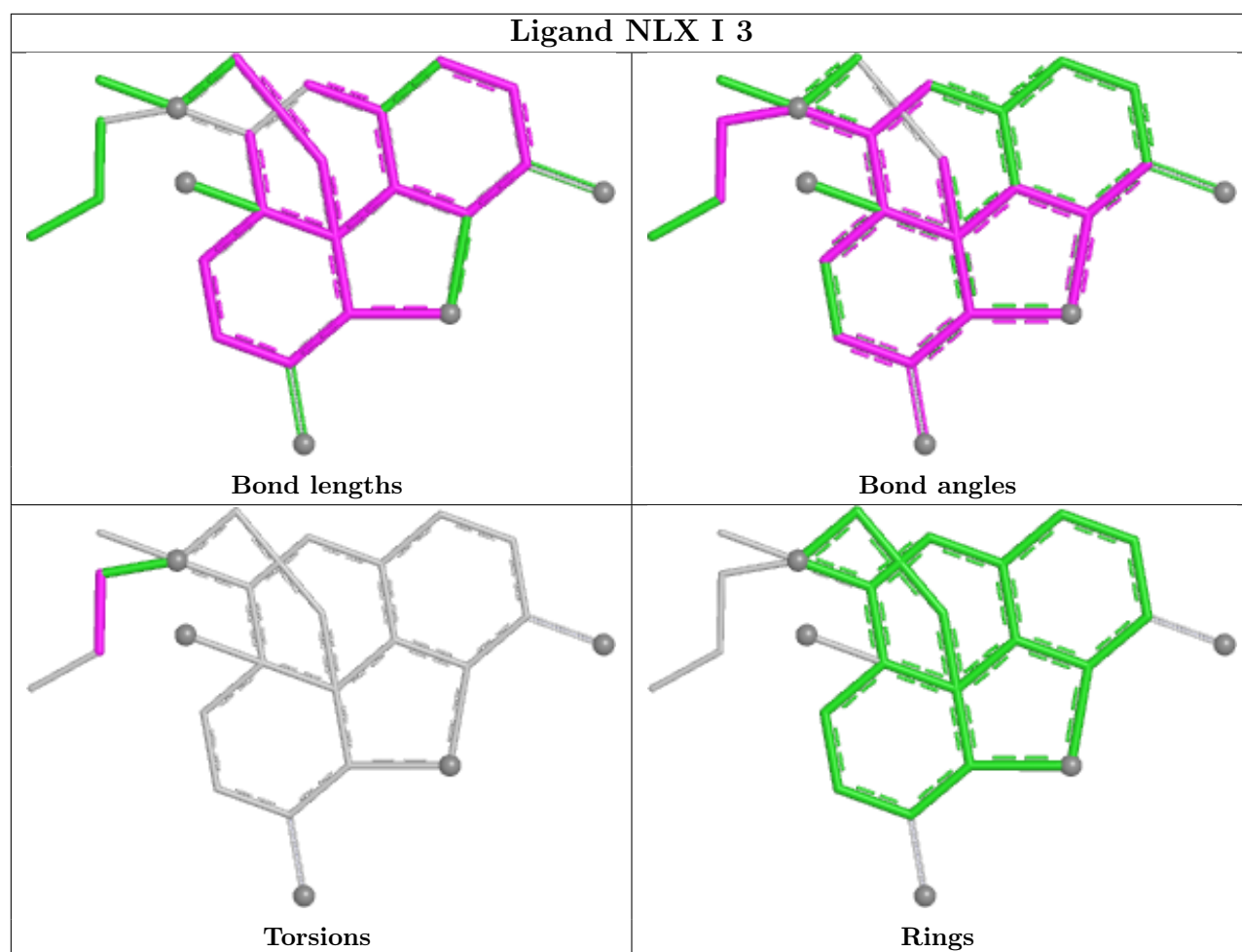


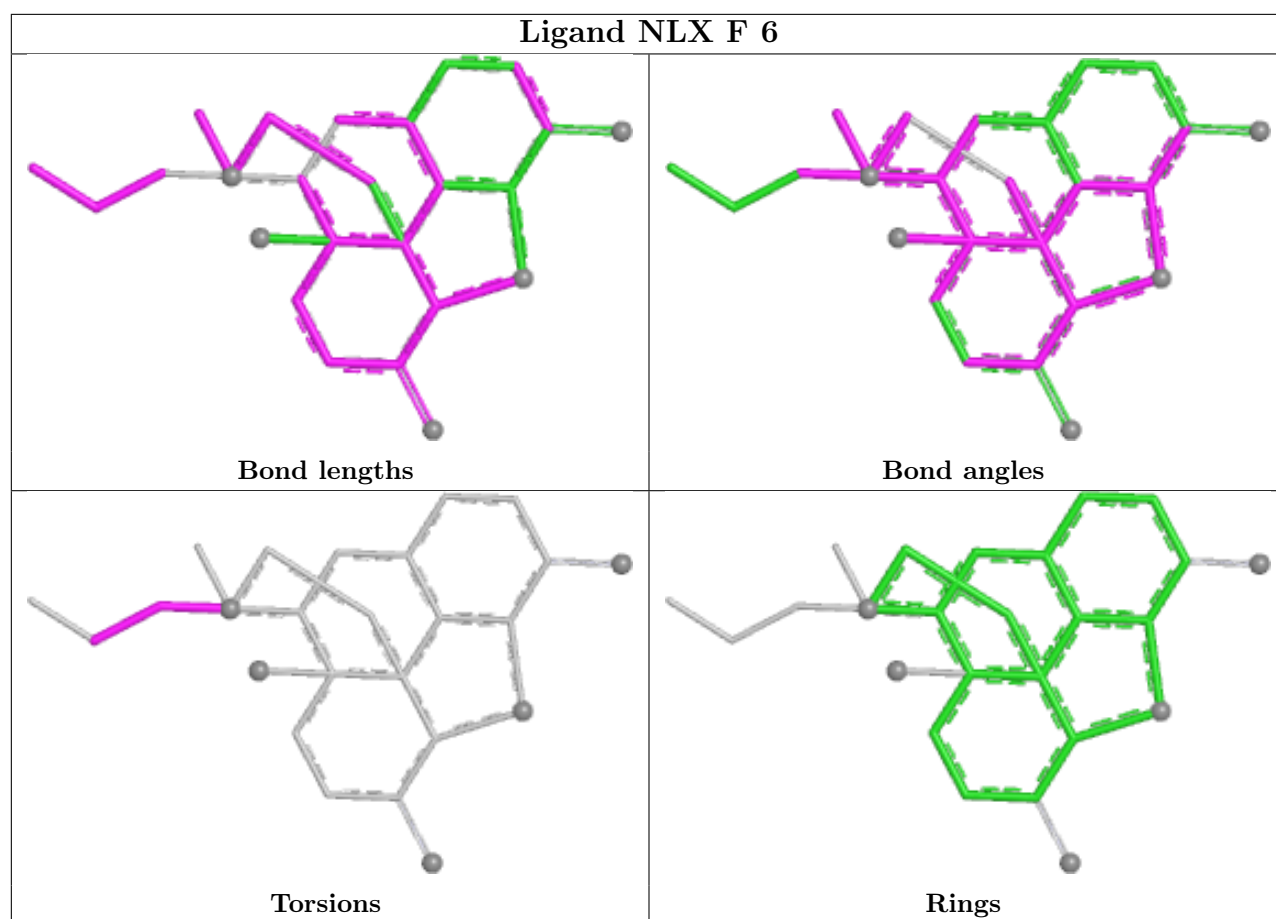
Ligand NLX L 6



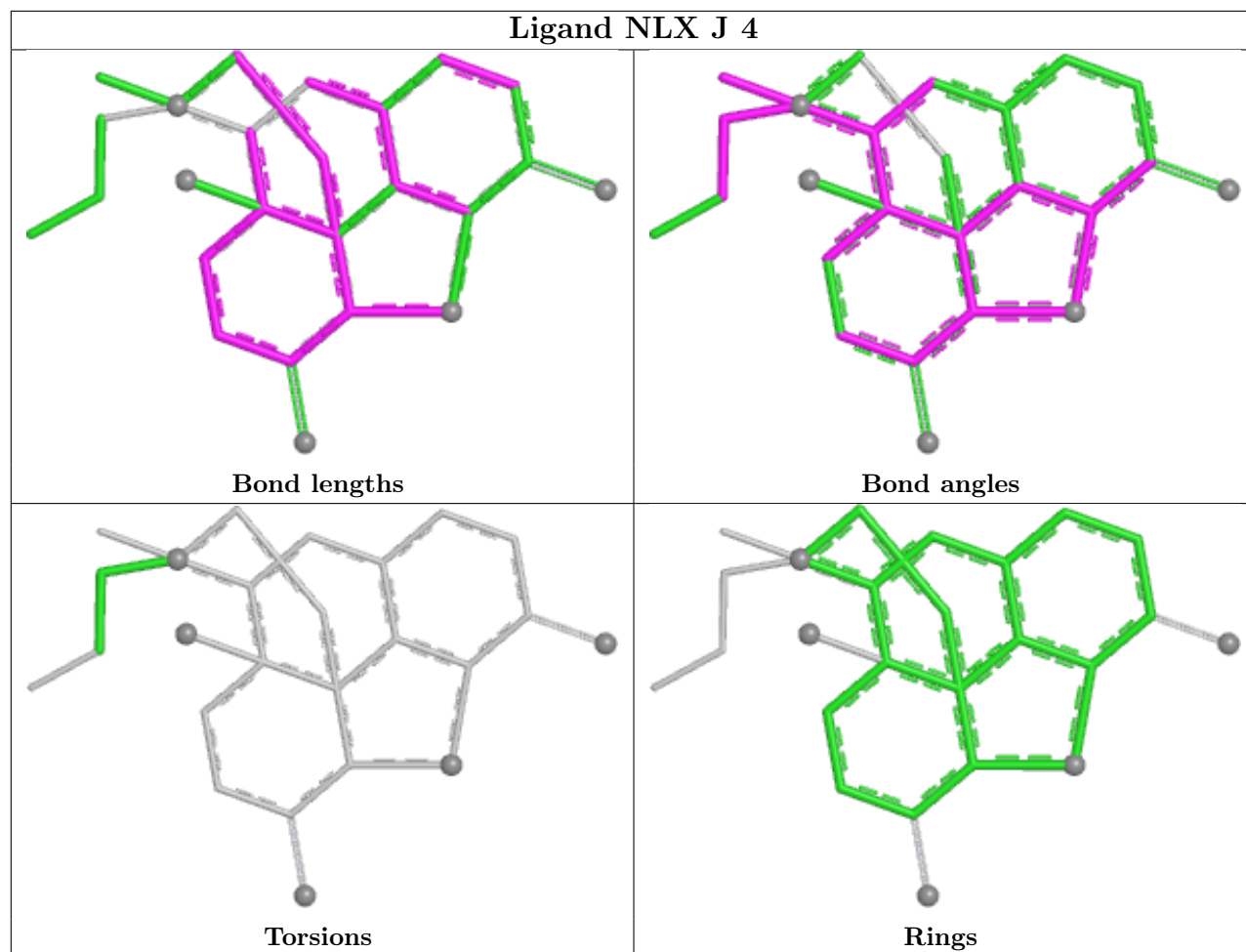
Ligand NLX D 4



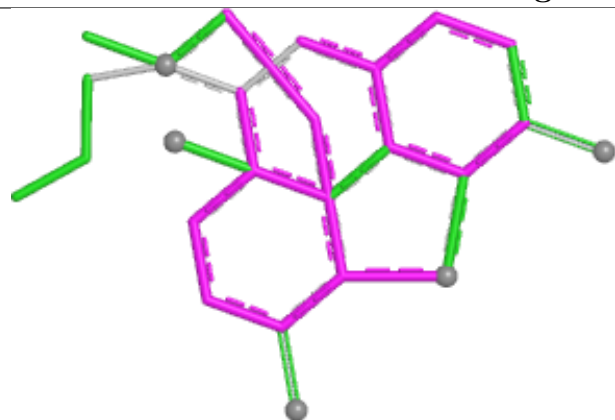




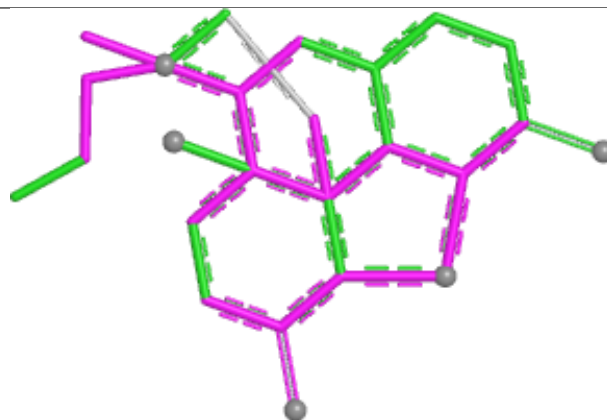
Ligand NLX J 4



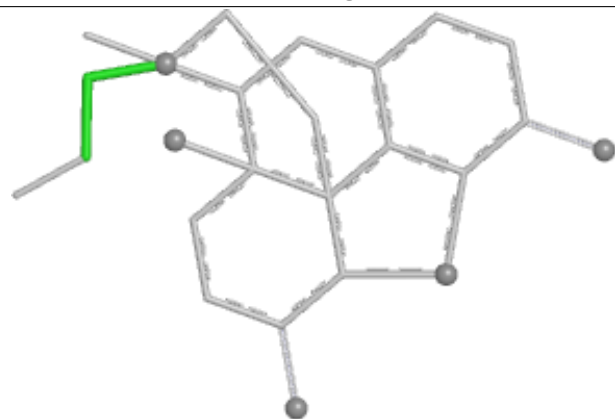
Ligand NLX E 5



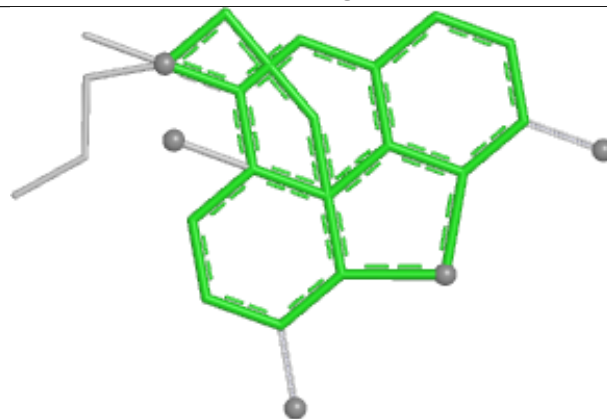
Bond lengths



Bond angles

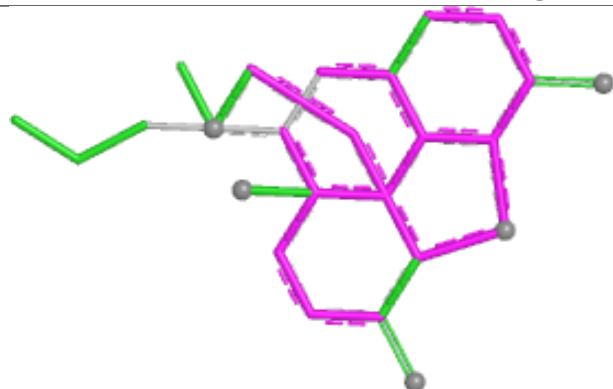


Torsions

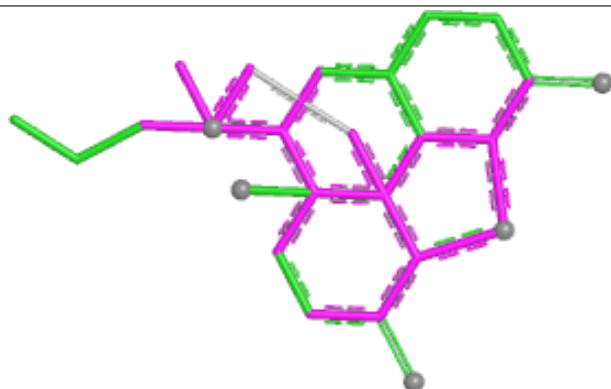


Rings

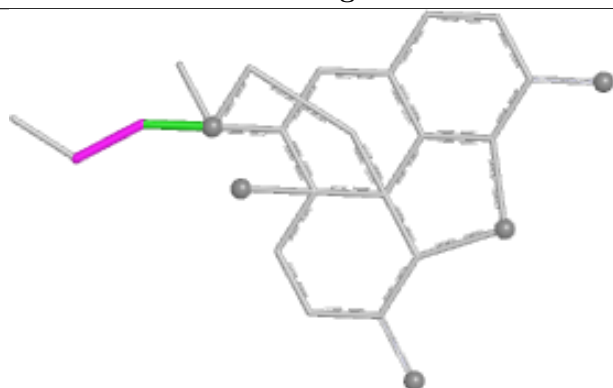
Ligand NLX C 3



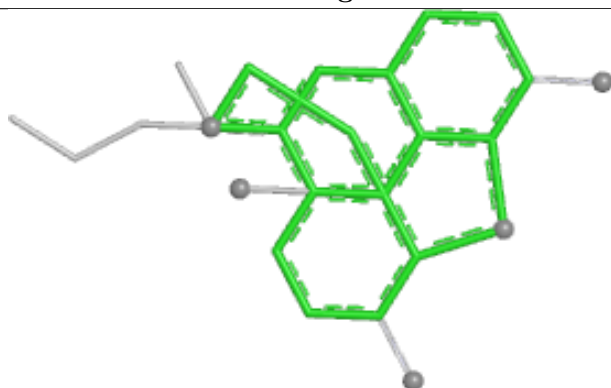
Bond lengths



Bond angles

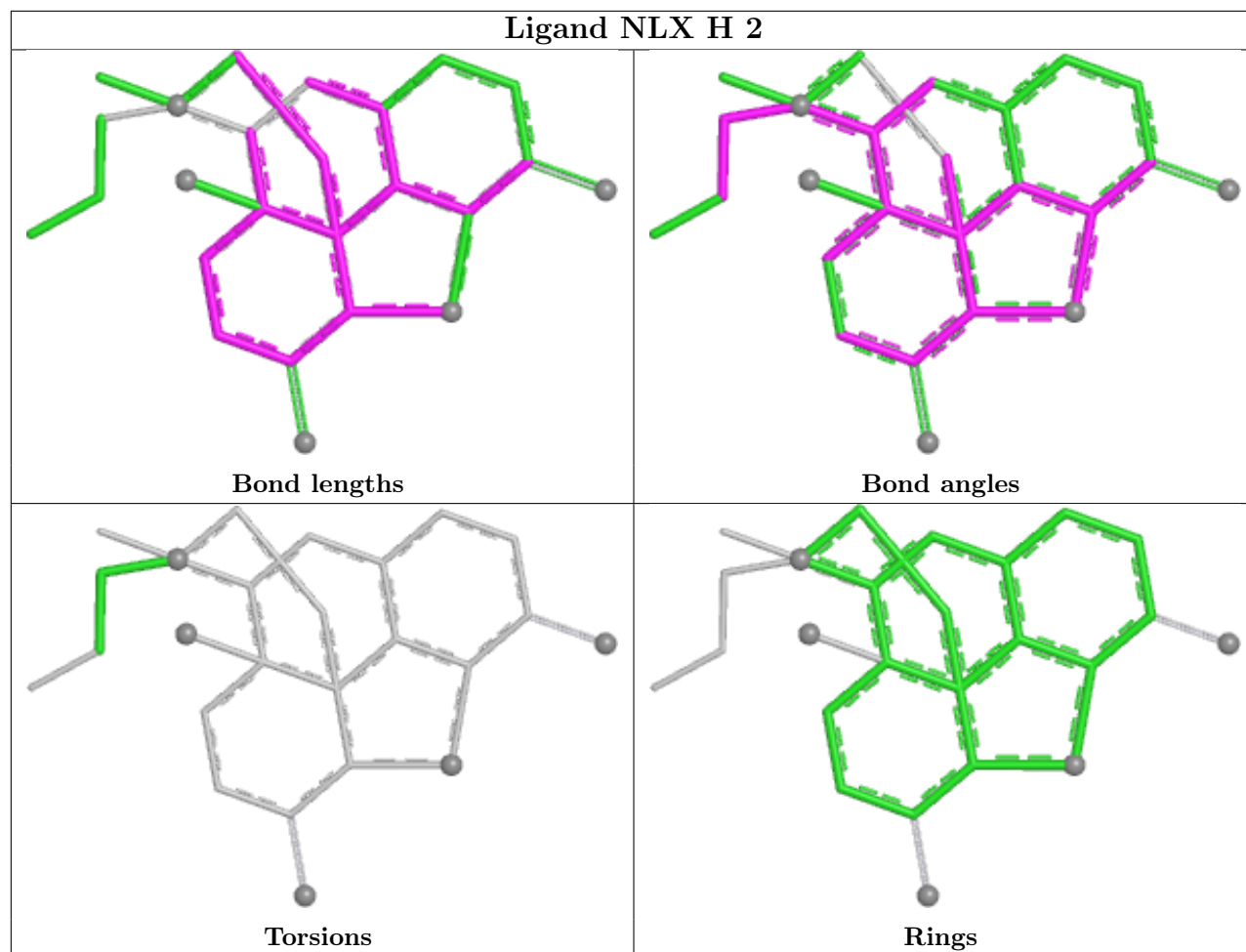


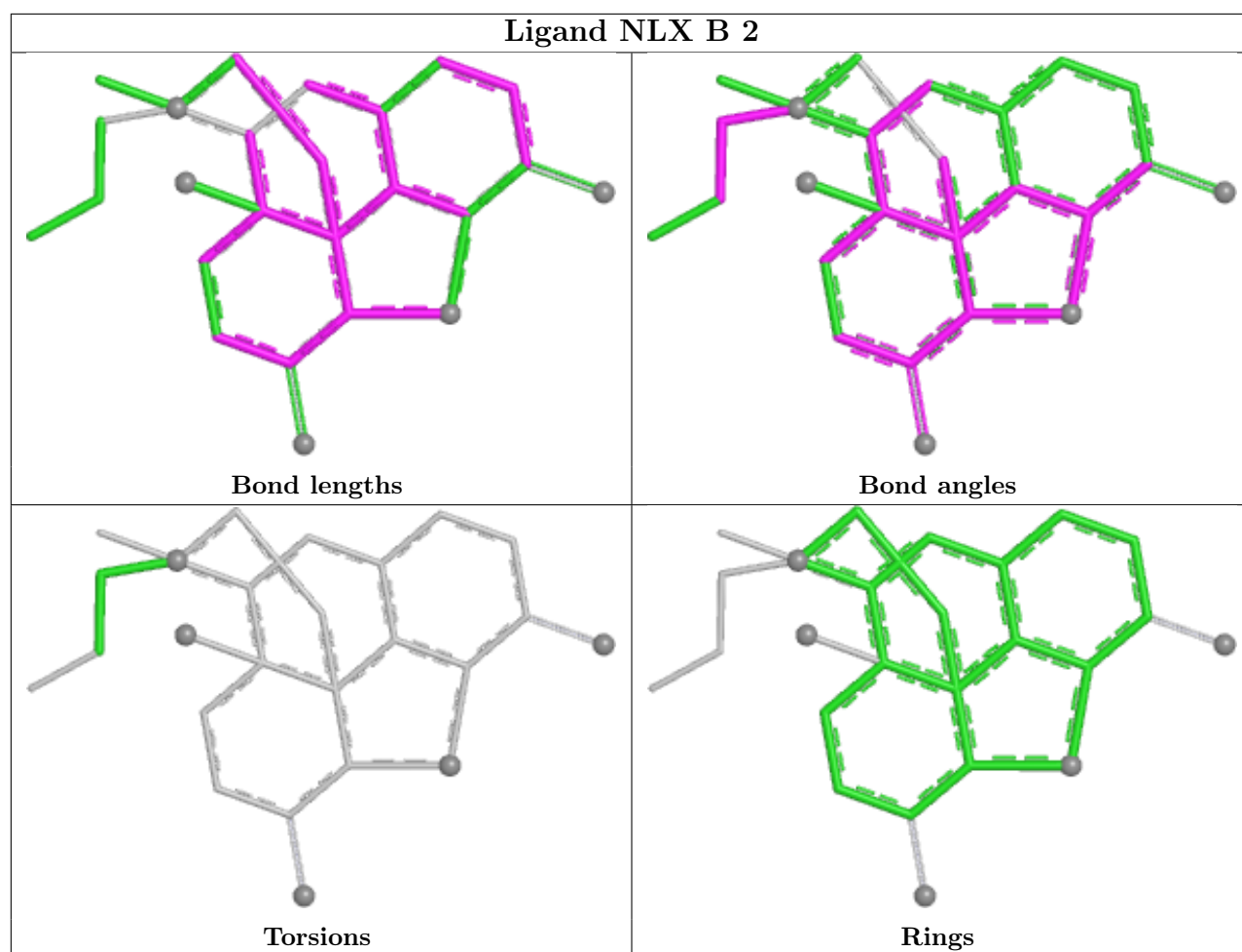
Torsions



Rings

Ligand NLX H 2





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.