



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 07:35 pm BST

PDB ID : 1V9P
Title : Crystal Structure Of Nad⁺-Dependent DNA Ligase
Authors : Lee, J.Y.; Chang, C.; Song, H.K.; Moon, J.; Yang, J.K.; Kim, H.K.; Kwon, S.K.; Suh, S.W.
Deposited on : 2004-01-27
Resolution : 2.90 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

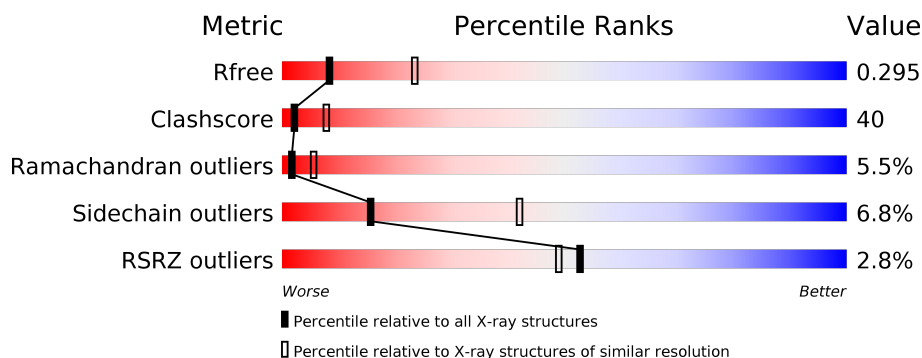
1 Overall quality at a glance

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))
R_{free}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	584	<div> <div>3%</div> <div> <div></div> <div>44%</div> <div>48%</div> <div>8%</div> </div> </div>
1	B	584	<div> <div>3%</div> <div> <div></div> <div>43%</div> <div>50%</div> <div>7%</div> </div> </div>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9768 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.

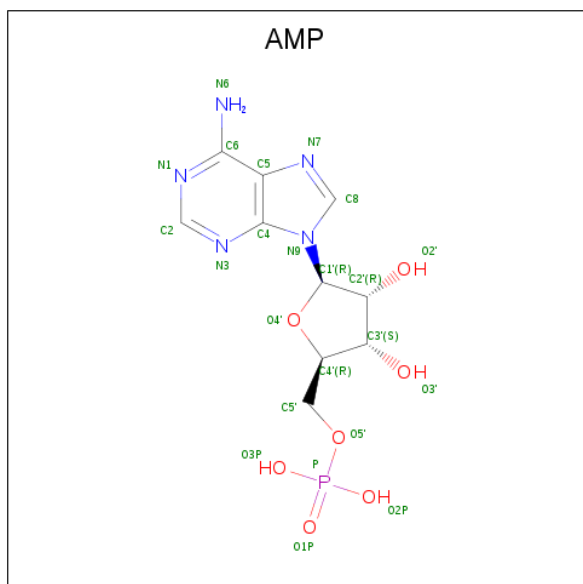
- Molecule 1 is a protein called DNA ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	584	Total	C	N	O	S	0	0	0
			4742	3000	860	871	11			
1	B	584	Total	C	N	O	S	0	0	0
			4742	3000	860	871	11			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Zn	0	0
			1	1		
2	A	1	Total	Zn	0	0
			1	1		

- Molecule 3 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: C₁₀H₁₄N₅O₇P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			22	10	5	6	1		
3	B	1	Total	C	N	O	P	0	0
			22	10	5	6	1		

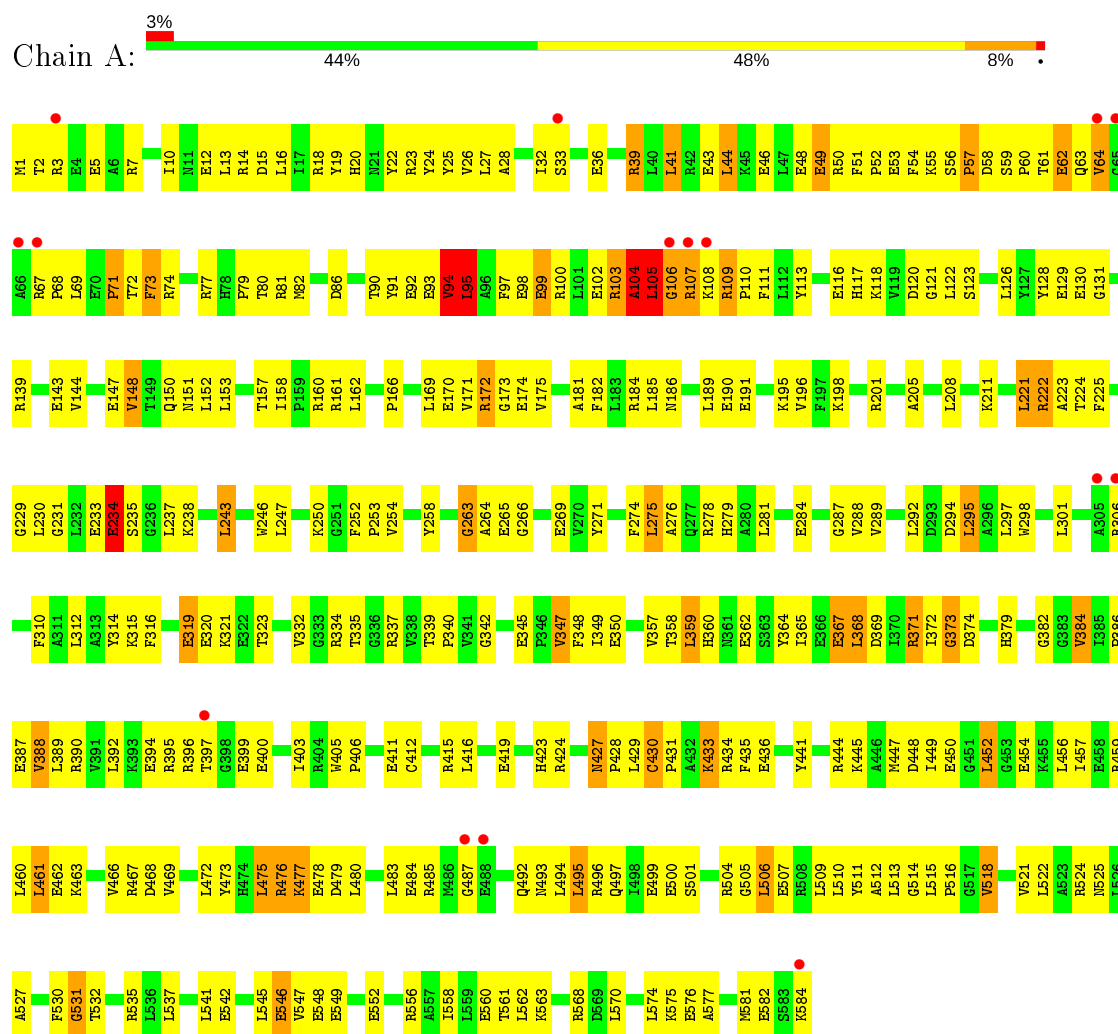
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	120	Total	O	0	0
			120	120		
4	B	118	Total	O	0	0
			118	118		

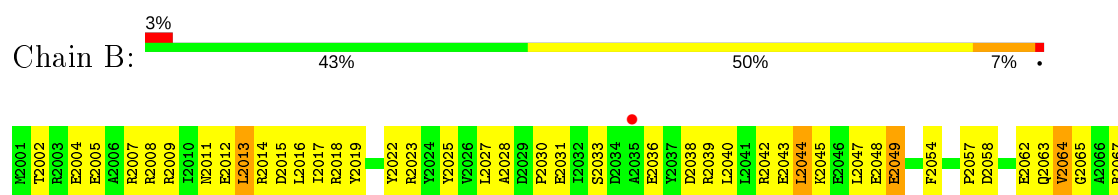
3 Residue-property plots

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

• Molecule 1: DNA ligase



• Molecule 1: DNA ligase



L2510	R2439	L2377	G2362	L2228	T2138	P2068
L2511	H2440	V2378	T2303	G2229	R2139	P2071
A2512	Y2441	H2379	T2304	L2230	G2140	F2072
L2513	A2442	R2380	A2305	G2231	D2141	R2073
G2514	S2443	G2383	R2306	L2232	G2142	R2074
L2515	R2444	R2384	A2307	E2233	E2143	E2075
V2516	K2445	V2385	R2308	E2234	V2144	V2076
A2446	M2447	L2386	R2309	S2235	G2145	V2077
E2517	G2451	E2387	Y2314	L2237	E2146	H2078
E2518	L2452	V2388	R2315	R2238	E2147	H2079
E2519	L2452	L2389	F2316	S2239	V2148	T2080
L2456	L2457	L2390	P2317	Q2240	T2149	
L2457	L2460	V2391	E2320	Y2241	Q2150	N2087
L2460	L2463	L2392	T2323	E2242	N2151	A2088
K2463	G2464	E2393	T2328	L2243	L2152	F2089
L2465	L2466	E2394	V2329	L2244	L2153	T2090
V2466	V2467	R2395	D2327	L2245	T2157	V2091
R2467	D2468	R2396	V2328	K2246	E2092	E2092
V2468	A2470	T2397	V2329	L2247	E2093	E2093
A2470	Y2473	G2398	F2330	K2250	V2094	L2095
Y2473	H2474	E2399	Q2331	F2252	L2162	A2096
H2474	L2475	E2400	V2332	G2251	P2166	F2097
L2475	R2476	R2401	G2333	F2253	L2169	E2098
R2476	R2477	P2402	R2334	V2254	E2170	E2099
R2477	E2478	L2403	T2335	E2255	L2171	R2100
E2478	D2479	R2404	G2336	H2256	G2173	L2101
D2479	E2484	V2405	R2337	G2257	R2174	E2102
E2484	V2485	K2413	F2340	Y2258	E2179	R2103
V2485	G2486	H2414	V2341	K2260	L2183	A2104
G2487	E2488	R2415	G2342	A2261	R2184	L2105
E2488	K2489	L2416	E2345	G2262	E2188	G2106
K2489	Q2492	V2417	P2346	A2264	L2189	R2107
Q2492	N2493	K2418	T2349	G2266	E2190	R2109
N2493	L2494	G2421	E2350	V2267	G2193	P2110
L2494	L2495	V2422	G2351	E2269	E2194	F2111
L2495	R2496	R2422	T2357	R2273	K2195	
R2496	Q2497	R2423	L2358	Q2277	V2196	L2112
Q2497	L2498	C2424	L2359	R2278	R2201	T2114
L2498	E2499	C2425	N2361	H2279	L2208	V2115
E2499	E2500	P2426	E2362	A2280	R2209	E2116
E2500	S2501	N2427	S2363	L2281	L2214	H2117
S2501	K2502	P2428	Y2364	P2282	R2214	K2118
K2502	H2503	L2429	L2368	F2283	E2284	V2119
H2503	R2504	C2430	D2369	E2285	A2285	G2121
R2504	K2505	P2431	T2370	D2286	L2221	L2122
K2505	G2505	A2432	R2371	L2292	R2222	S2123
G2505	L2506	R2433	T2372	L2298	A2223	V2124
L2506	E2507	E2434	G2373	W2298	T2224	L2126
E2507	R2508	F2435	D2374	L2301	F2225	Y2127
R2508	L2509	A2437	V2375		Y2226	E2128
L2509		I2438	V2376		A2227	E2129

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	89.21Å 117.33Å 97.48Å 90.00° 115.09° 90.00°	Depositor
Resolution (Å)	19.93 – 2.90 24.75 – 2.88	Depositor EDS
% Data completeness (in resolution range)	89.4 (19.93-2.90) 94.4 (24.75-2.88)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.48 (at 2.89Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.232 , 0.293 0.238 , 0.295	Depositor DCC
R_{free} test set	3869 reflections (9.94%)	wwPDB-VP
Wilson B-factor (Å ²)	53.4	Xtriage
Anisotropy	0.238	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 61.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.022 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	9768	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.47	2/4832 (0.0%)	0.75	7/6514 (0.1%)
1	B	0.42	2/4832 (0.0%)	0.70	5/6514 (0.1%)
All	All	0.45	4/9664 (0.0%)	0.72	12/13028 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	359	LEU	N-CA	-6.58	1.33	1.46
1	B	2120	ASP	C-N	-6.48	1.21	1.33
1	A	487	GLY	N-CA	-5.20	1.38	1.46
1	B	2360	HIS	C-N	-5.09	1.22	1.34

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	359	LEU	CB-CA-C	11.56	132.16	110.20
1	B	2360	HIS	CA-C-N	9.32	137.70	117.20
1	A	359	LEU	N-CA-C	-8.49	88.08	111.00
1	A	94	VAL	CB-CA-C	-7.80	96.57	111.40
1	B	2360	HIS	N-CA-C	7.72	131.85	111.00
1	B	2360	HIS	O-C-N	-6.71	111.97	122.70
1	A	104	ALA	C-N-CA	6.02	136.74	121.70
1	B	2360	HIS	C-N-CA	-6.00	106.71	121.70
1	B	2120	ASP	C-N-CA	-5.88	109.96	122.30
1	A	229	GLY	N-CA-C	-5.58	99.15	113.10
1	A	233	GLU	CA-C-N	-5.52	105.05	117.20
1	A	95	LEU	N-CA-C	-5.05	97.37	111.00

There are no chirality outliers.

There are no planarity outliers.

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	4742	0	4797	388	0
1	B	4742	0	4794	369	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	22	0	12	2	0
3	B	22	0	12	1	0
4	A	120	0	0	15	0
4	B	118	0	0	6	0
All	All	9768	0	9615	757	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 40.

All (757) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2360:HIS:O	1:B:2361:ASN:HB3	1.37	1.11
1:A:10:ILE:HG23	1:A:14:ARG:NH1	1.68	1.09
1:A:166:PRO:CG	1:A:234:GLU:HB3	1.88	1.03
1:A:537:LEU:HD22	1:A:568:ARG:HE	1.24	1.02
1:B:2360:HIS:O	1:B:2361:ASN:CB	2.00	1.00
1:A:166:PRO:HG3	1:A:234:GLU:HB3	1.45	0.98
1:B:2077:ARG:HA	1:B:2143:GLU:O	1.65	0.94
1:A:144:VAL:HB	4:A:1002:HOH:O	1.68	0.94
1:B:2057:PRO:HA	1:B:2062:GLU:HG3	1.52	0.92
1:B:2362:GLU:HG3	1:B:2421:LYS:O	1.71	0.91
1:A:427:ASN:ND2	1:A:429:LEU:H	1.69	0.90
1:A:99:GLU:HA	1:A:102:GLU:HG3	1.53	0.90
1:B:2118:LYS:HZ1	1:B:2286:ASP:HB2	1.35	0.90
1:A:427:ASN:HD22	1:A:429:LEU:H	1.13	0.89
1:B:2105:LEU:HG	1:B:2106:GLY:N	1.88	0.89
1:B:2169:LEU:HD11	1:B:2228:LEU:HD22	1.55	0.89
1:A:319:GLU:HG2	1:A:350:GLU:HG3	1.56	0.87
1:A:537:LEU:HD22	1:A:568:ARG:NE	1.90	0.86
1:A:10:ILE:HG23	1:A:14:ARG:HH12	1.34	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2445:LYS:HD3	1:B:2520:GLU:OE1	1.76	0.85
1:A:80:THR:HG23	1:A:230:LEU:CD2	2.07	0.84
1:B:2478:GLU:HG3	1:B:2495:LEU:HD13	1.59	0.84
1:A:80:THR:HG23	1:A:230:LEU:HD22	1.58	0.84
1:A:449:ILE:HG21	1:A:452:LEU:HD23	1.59	0.84
1:A:102:GLU:HA	4:A:1225:HOH:O	1.76	0.84
1:A:525:ASN:HD22	1:A:548:GLU:HB3	1.40	0.83
1:B:2074:ARG:NH1	1:B:2076:VAL:HG22	1.93	0.83
1:B:2033:SER:OG	1:B:2036:GLU:HG3	1.80	0.82
1:A:20:HIS:HA	1:A:23:ARG:HB2	1.62	0.82
1:A:105:LEU:HD22	1:A:106:GLY:H	1.44	0.81
1:A:126:LEU:HB3	1:A:128:TYR:HE1	1.45	0.81
1:B:2014:ARG:O	1:B:2018:ARG:HG3	1.80	0.81
1:A:126:LEU:HD11	1:A:152:LEU:HD13	1.63	0.80
1:A:44:LEU:HD11	1:A:60:PRO:HD2	1.64	0.80
1:B:2357:VAL:CG2	1:B:2387:GLU:HA	2.11	0.80
1:A:340:PRO:HD2	1:A:360:HIS:O	1.82	0.80
1:B:2515:LEU:O	1:B:2518:VAL:HG12	1.83	0.79
1:A:406:PRO:O	1:A:416:LEU:HD12	1.83	0.79
1:A:123:SER:HB2	1:A:139:ARG:HB2	1.64	0.78
1:B:2023:ARG:HH11	1:B:2031:GLU:HG3	1.49	0.78
1:A:44:LEU:HD22	1:A:48:GLU:OE2	1.84	0.78
1:A:94:VAL:HG12	1:A:94:VAL:O	1.81	0.77
1:B:2556:ARG:HB2	1:B:2556:ARG:NH2	1.98	0.77
1:A:196:VAL:HG21	1:A:360:HIS:CE1	2.20	0.77
1:A:105:LEU:HD21	1:A:108:LYS:O	1.83	0.77
1:A:501:SER:HA	1:A:504:ARG:HE	1.50	0.77
1:A:122:LEU:HD11	1:A:201:ARG:O	1.84	0.77
1:A:525:ASN:ND2	1:A:548:GLU:HB3	2.00	0.76
1:A:427:ASN:HD22	1:A:429:LEU:N	1.83	0.76
1:B:2122:LEU:HD13	1:B:2208:LEU:HD22	1.67	0.76
1:B:2125:ASN:HD21	1:B:2172:ARG:HE	1.32	0.76
1:A:507:GLU:HG3	1:A:527:ALA:HB3	1.67	0.76
1:B:2036:GLU:HG2	1:B:2039:ARG:NH2	2.01	0.76
1:B:2105:LEU:HD11	1:B:2108:LYS:H	1.50	0.76
1:B:2105:LEU:HD22	1:B:2111:PHE:CZ	2.20	0.75
1:A:515:LEU:HB2	1:A:518:VAL:CG1	2.16	0.75
1:A:369:ASP:OD2	1:A:371:ARG:HD2	1.85	0.75
1:A:1:MET:HB2	1:A:5:GLU:OE2	1.86	0.75
1:B:2368:LEU:HD12	1:B:2390:ARG:HA	1.69	0.75
1:A:319:GLU:HG3	1:A:349:ILE:HG23	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:LYS:HG2	1:A:289:VAL:HG23	1.70	0.74
1:B:2320:GLU:HB3	1:B:2377:LEU:HD21	1.69	0.74
1:A:541:LEU:HD21	1:A:556:ARG:NH1	2.02	0.74
1:B:2105:LEU:HD22	1:B:2111:PHE:HZ	1.53	0.73
1:A:103:ARG:O	1:A:104:ALA:HB2	1.88	0.73
1:A:459:ARG:HH11	1:A:462:GLU:HB3	1.54	0.72
1:B:2383:GLY:HA2	4:B:1020:HOH:O	1.89	0.72
1:B:2067:ARG:CG	1:B:2068:PRO:HD2	2.18	0.72
1:B:2417:VAL:HG22	1:B:2418:LYS:H	1.54	0.72
1:B:2109:ARG:HB3	1:B:2110:PRO:HD3	1.71	0.72
1:A:515:LEU:HB2	1:A:518:VAL:HG11	1.71	0.72
1:B:2193:GLY:HA3	1:B:2421:LYS:HB2	1.72	0.72
1:B:2171:VAL:HG21	1:B:2252:PHE:CZ	2.25	0.72
1:A:320:GLU:C	1:A:321:LYS:HD2	2.10	0.71
1:B:2494:LEU:HA	1:B:2497:GLN:HE21	1.54	0.71
1:B:2058:ASP:OD2	1:B:2147:GLU:HG3	1.91	0.71
1:B:2384:VAL:HG13	1:B:2385:ILE:H	1.53	0.71
1:A:100:ARG:O	1:A:103:ARG:HG2	1.91	0.71
1:B:2376:VAL:HG12	1:B:2391:VAL:HA	1.71	0.71
1:A:118:LYS:NZ	3:A:700:AMP:P	2.64	0.70
1:B:2162:LEU:HD21	1:B:2252:PHE:CE2	2.25	0.70
1:A:358:THR:C	1:A:359:LEU:O	2.18	0.70
1:A:358:THR:OG1	1:A:359:LEU:O	2.08	0.70
1:A:105:LEU:CD2	1:A:106:GLY:H	2.05	0.70
1:A:14:ARG:HG2	1:A:60:PRO:CD	2.22	0.70
1:A:515:LEU:HD23	1:A:561:THR:HG21	1.74	0.70
1:A:445:LYS:HB3	1:A:511:TYR:CE2	2.27	0.69
1:A:278:ARG:NH1	1:A:316:PHE:HB3	2.07	0.69
1:B:2036:GLU:O	1:B:2040:LEU:HG	1.93	0.69
1:B:2125:ASN:ND2	1:B:2172:ARG:NE	2.40	0.69
1:B:2008:ARG:HA	1:B:2011:ASN:HD22	1.57	0.69
1:B:2121:GLY:O	1:B:2201:ARG:HG3	1.93	0.69
1:A:41:LEU:HD21	1:A:64:VAL:HG11	1.74	0.69
1:A:278:ARG:HG2	1:A:279:HIS:CD2	2.28	0.69
1:A:449:ILE:CG2	1:A:452:LEU:HD23	2.22	0.68
1:A:524:ARG:HB2	1:A:524:ARG:NH1	2.09	0.68
1:B:2105:LEU:HD21	1:B:2108:LYS:N	2.08	0.68
1:A:445:LYS:HB3	1:A:511:TYR:HE2	1.57	0.68
1:B:2357:VAL:HG23	1:B:2387:GLU:HA	1.74	0.68
1:B:2125:ASN:HD21	1:B:2172:ARG:NE	1.92	0.68
1:B:2140:GLY:HA3	1:B:2144:VAL:O	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2195:LYS:HE3	1:B:2364:TYR:CD1	2.28	0.67
1:A:14:ARG:HG2	1:A:60:PRO:HD3	1.77	0.67
1:B:2038:ASP:O	1:B:2042:ARG:HG3	1.95	0.67
1:A:506:LEU:HD22	1:A:510:LEU:HG	1.77	0.67
1:B:2015:ASP:OD2	1:B:2161:ARG:NH1	2.26	0.67
1:A:71:PRO:HG2	1:A:73:PHE:HE2	1.59	0.67
1:A:332:VAL:CG1	1:A:411:GLU:HG3	2.25	0.67
1:A:46:GLU:O	1:A:50:ARG:HG2	1.94	0.67
1:B:2039:ARG:HG3	1:B:2042:ARG:NH2	2.10	0.67
1:B:2196:VAL:HG21	1:B:2360:HIS:CD2	2.30	0.67
1:B:2122:LEU:CD1	1:B:2208:LEU:HD22	2.24	0.66
1:A:518:VAL:HG13	1:A:518:VAL:O	1.93	0.66
1:A:118:LYS:HZ3	3:A:700:AMP:P	2.18	0.66
1:B:2384:VAL:HG22	1:B:2385:ILE:N	2.10	0.66
1:A:61:THR:HA	1:A:64:VAL:HG13	1.76	0.66
1:A:57:PRO:HA	1:A:62:GLU:HG3	1.76	0.66
1:B:2190:GLU:HG2	1:B:2337:ARG:NH1	2.10	0.66
1:B:2469:VAL:HG23	1:B:2574:LEU:HD21	1.75	0.66
1:A:49:GLU:OE1	1:A:55:LYS:HE2	1.96	0.66
1:B:2067:ARG:HG2	1:B:2068:PRO:HD2	1.78	0.66
1:A:427:ASN:ND2	1:A:429:LEU:N	2.44	0.65
1:B:2101:LEU:HD21	1:B:2292:LEU:HD13	1.77	0.65
1:B:2105:LEU:CD1	1:B:2108:LYS:HB2	2.26	0.65
1:B:2349:ILE:CG2	1:B:2380:LYS:HE3	2.26	0.65
1:B:2172:ARG:HH21	1:B:2172:ARG:HG2	1.60	0.65
1:B:2118:LYS:NZ	1:B:2286:ASP:HB2	2.10	0.65
1:B:2510:LEU:HD12	1:B:2527:ALA:HB2	1.78	0.65
1:A:397:THR:HG23	1:A:399:GLU:H	1.61	0.65
1:B:2073:PHE:HB3	1:B:2146:GLU:OE1	1.97	0.65
1:A:39:ARG:HA	1:A:39:ARG:HE	1.60	0.64
1:A:452:LEU:HD12	1:A:457:ILE:HG12	1.77	0.64
1:A:463:LYS:HE2	4:A:1145:HOH:O	1.96	0.64
1:B:2057:PRO:CA	1:B:2062:GLU:HG3	2.27	0.64
1:A:175:VAL:HG22	1:A:223:ALA:HB2	1.78	0.64
1:A:195:LYS:HD2	1:A:367:GLU:HG2	1.80	0.64
1:A:93:GLU:O	1:A:94:VAL:CB	2.44	0.64
1:B:2141:ASP:HB3	4:B:1006:HOH:O	1.96	0.64
1:A:332:VAL:HG12	1:A:411:GLU:HG3	1.79	0.64
1:B:2079:PRO:HB2	1:B:2170:GLU:OE2	1.97	0.64
1:A:548:GLU:O	1:A:549:GLU:HB2	1.98	0.64
1:B:2504:ARG:HD2	1:B:2508:ARG:HH21	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2142:GLY:O	1:B:2143:GLU:CB	2.45	0.63
1:B:2530:PHE:O	1:B:2532:THR:N	2.29	0.63
1:A:14:ARG:HH11	1:A:14:ARG:HG3	1.61	0.63
1:A:278:ARG:HH11	1:A:316:PHE:HB3	1.64	0.63
1:B:2460:LEU:HD23	1:B:2465:LEU:HD12	1.79	0.63
1:B:2556:ARG:HB2	1:B:2556:ARG:HH21	1.62	0.63
1:B:2405:TRP:CB	1:B:2423:HIS:HD1	2.12	0.63
1:A:71:PRO:HB3	1:A:150:GLN:HB2	1.81	0.63
1:B:2039:ARG:HG3	1:B:2042:ARG:HH21	1.63	0.63
1:A:152:LEU:HD23	1:A:208:LEU:HD11	1.79	0.63
1:B:2080:THR:CG2	1:B:2230:LEU:HD23	2.29	0.63
1:B:2120:ASP:OD2	1:B:2284:GLU:HB3	1.98	0.63
1:A:16:LEU:HD11	1:A:161:ARG:HH22	1.63	0.62
1:A:457:ILE:O	1:A:461:LEU:HD23	1.99	0.62
1:A:93:GLU:O	1:A:94:VAL:HB	2.00	0.62
1:A:166:PRO:CG	1:A:234:GLU:CB	2.72	0.62
1:A:335:THR:HG23	1:A:337:ARG:H	1.62	0.62
1:A:109:ARG:HB3	1:A:110:PRO:HD3	1.80	0.62
1:B:2328:VAL:HG22	1:B:2328:VAL:O	1.99	0.62
1:A:372:ILE:O	1:A:374:ASP:N	2.33	0.62
1:B:2142:GLY:O	1:B:2143:GLU:HB2	1.98	0.62
1:B:2222:ARG:HG2	1:B:2222:ARG:HH21	1.65	0.62
1:A:198:LYS:HE3	1:A:364:TYR:OH	2.00	0.62
1:A:542:GLU:O	1:A:546:GLU:HG3	2.00	0.62
1:B:2357:VAL:HG21	1:B:2387:GLU:HA	1.81	0.62
1:B:2361:ASN:O	1:B:2362:GLU:C	2.38	0.62
1:A:61:THR:O	1:A:63:GLN:N	2.33	0.61
1:B:2077:ARG:NH1	1:B:2143:GLU:HB3	2.15	0.61
1:A:493:ASN:O	1:A:496:ARG:HG2	2.01	0.61
1:B:2148:VAL:HG22	1:B:2148:VAL:O	1.99	0.61
1:B:2556:ARG:HH21	1:B:2556:ARG:CB	2.13	0.61
1:B:2099:GLU:O	1:B:2102:GLU:HB2	2.01	0.61
1:B:2316:PHE:HB3	1:B:2317:PRO:HD2	1.83	0.61
1:B:2105:LEU:CG	1:B:2106:GLY:N	2.60	0.61
1:B:2172:ARG:NH2	1:B:2172:ARG:HG2	2.16	0.61
1:A:33:SER:HB2	1:A:36:GLU:H	1.65	0.61
1:B:2122:LEU:HD11	1:B:2208:LEU:CD2	2.31	0.61
1:B:2518:VAL:HG13	1:B:2518:VAL:O	2.01	0.61
1:A:14:ARG:NH1	1:A:44:LEU:HD21	2.16	0.61
1:A:10:ILE:HD12	1:A:54:PHE:HD1	1.66	0.61
1:B:2094:VAL:O	1:B:2097:PHE:HB3	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:LEU:HB3	1:A:128:TYR:CE1	2.33	0.60
1:B:2122:LEU:CD1	1:B:2208:LEU:CD2	2.79	0.60
1:A:441:TYR:CE1	1:A:469:VAL:HG11	2.37	0.60
1:B:2184:ARG:O	1:B:2188:GLU:HG3	2.02	0.60
1:A:71:PRO:HG2	1:A:73:PHE:CE2	2.36	0.60
1:A:172:ARG:HG2	1:A:172:ARG:HH21	1.67	0.60
1:A:237:LEU:CD1	1:A:243:LEU:HD12	2.32	0.60
1:A:319:GLU:CG	1:A:350:GLU:HG3	2.30	0.60
1:B:2222:ARG:NH2	1:B:2222:ARG:HG2	2.15	0.60
1:B:2065:GLY:C	1:B:2067:ARG:H	2.04	0.60
1:B:2417:VAL:HG22	1:B:2418:LYS:N	2.17	0.60
1:A:16:LEU:HD11	1:A:161:ARG:NH2	2.15	0.60
1:A:372:ILE:HG22	1:A:373:GLY:N	2.17	0.60
1:A:522:LEU:HD13	1:A:522:LEU:O	2.01	0.60
1:B:2240:GLN:NE2	1:B:2243:LEU:HD13	2.16	0.60
1:A:56:SER:C	1:A:58:ASP:H	2.05	0.59
1:B:2228:LEU:HD12	1:B:2232:LEU:HD23	1.84	0.59
1:B:2240:GLN:HE21	1:B:2243:LEU:HD13	1.66	0.59
1:A:57:PRO:HG2	1:A:74:ARG:CD	2.32	0.59
1:A:67:ARG:HB3	1:A:68:PRO:HD2	1.85	0.59
1:B:2002:THR:HG23	1:B:2005:GLU:H	1.67	0.59
1:B:2013:LEU:O	1:B:2017:ILE:HG13	2.01	0.59
1:B:2072:THR:HG22	4:B:1094:HOH:O	2.02	0.59
1:A:105:LEU:HD21	1:A:108:LYS:C	2.22	0.59
1:A:184:ARG:NH1	4:A:1154:HOH:O	2.34	0.59
1:A:166:PRO:HB3	1:A:234:GLU:CG	2.32	0.59
1:A:284:GLU:OE2	1:A:382:GLY:HA2	2.01	0.59
1:B:2349:ILE:HD11	1:B:2378:VAL:HG13	1.84	0.59
1:B:2506:LEU:HB3	1:B:2527:ALA:HB1	1.84	0.59
1:A:103:ARG:O	1:A:104:ALA:CB	2.51	0.59
1:A:148:VAL:HG22	1:A:151:ASN:HB2	1.84	0.59
1:A:41:LEU:HD21	1:A:64:VAL:CG1	2.33	0.58
1:B:2103:ARG:O	1:B:2104:ALA:HB3	2.02	0.58
1:A:459:ARG:HE	1:A:459:ARG:HA	1.67	0.58
1:A:16:LEU:CD1	1:A:161:ARG:HH22	2.17	0.58
1:B:2224:THR:O	1:B:2224:THR:HG23	2.02	0.58
1:B:2349:ILE:HG22	1:B:2380:LYS:HE3	1.85	0.58
1:B:2496:ARG:HH11	1:B:2496:ARG:HG3	1.69	0.58
1:A:82:MET:HG2	1:A:172:ARG:NH2	2.18	0.58
1:B:2122:LEU:O	1:B:2123:SER:C	2.41	0.58
1:B:2179:ILE:O	1:B:2183:LEU:HG	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:ALA:HB3	4:A:1207:HOH:O	2.03	0.58
1:A:441:TYR:CZ	1:A:447:MET:HG3	2.38	0.58
1:B:2359:LEU:O	1:B:2361:ASN:N	2.37	0.58
1:A:172:ARG:HG2	1:A:172:ARG:NH2	2.19	0.58
1:B:2533:MET:HE3	1:B:2571:VAL:HG21	1.85	0.58
1:A:98:GLU:OE2	1:A:263:GLY:HA2	2.02	0.57
1:B:2123:SER:HA	1:B:2174:GLU:HG2	1.85	0.57
1:B:2190:GLU:HG3	1:B:2360:HIS:HB3	1.85	0.57
1:B:2157:THR:HG21	1:B:2222:ARG:HH22	1.69	0.57
1:A:12:GLU:O	1:A:16:LEU:HD13	2.03	0.57
1:A:494:LEU:HD23	1:A:494:LEU:O	2.03	0.57
1:B:2452:LEU:HD12	1:B:2456:LEU:HD23	1.86	0.57
1:A:298:TRP:O	1:A:301:LEU:O	2.23	0.57
1:B:2362:GLU:OE1	1:B:2422:VAL:HA	2.05	0.57
1:A:478:GLU:OE1	1:A:492:GLN:HG2	2.04	0.57
1:B:2426:PRO:O	1:B:2428:PRO:HD3	2.05	0.57
1:A:186:ASN:OD1	1:A:196:VAL:HB	2.04	0.57
1:A:173:GLY:HA3	1:A:225:PHE:CD1	2.39	0.57
1:B:2122:LEU:O	1:B:2122:LEU:HD22	2.05	0.57
1:B:2548:GLU:OE2	1:B:2549:GLU:HG2	2.04	0.57
1:B:2105:LEU:HD11	1:B:2108:LYS:HB2	1.87	0.57
1:B:2150:GLN:HE21	1:B:2150:GLN:CA	2.18	0.57
1:A:507:GLU:HG3	1:A:527:ALA:CB	2.34	0.57
1:A:469:VAL:HG12	1:A:574:LEU:HD21	1.84	0.57
1:A:58:ASP:CG	1:A:74:ARG:HE	2.08	0.57
1:B:2148:VAL:HG22	1:B:2151:ASN:HB2	1.85	0.56
1:A:113:TYR:HD2	1:A:292:LEU:HA	1.70	0.56
1:B:2194:GLU:O	1:B:2361:ASN:ND2	2.36	0.56
1:B:2157:THR:HB	1:B:2253:PRO:HB3	1.86	0.56
1:B:2162:LEU:HD21	1:B:2252:PHE:CZ	2.40	0.56
1:B:2087:ASN:ND2	1:B:2315:LYS:HD2	2.19	0.56
1:A:247:LEU:O	1:A:252:PHE:HB2	2.06	0.56
1:A:484:GLU:O	1:A:485:ARG:HB2	2.06	0.56
1:B:2002:THR:HG22	1:B:2005:GLU:CG	2.35	0.56
1:B:2337:ARG:HD2	1:B:2422:VAL:HG11	1.86	0.56
1:B:2563:LYS:HD3	4:B:1176:HOH:O	2.06	0.56
1:B:2122:LEU:O	1:B:2124:VAL:HG13	2.05	0.56
1:A:237:LEU:HD12	1:A:243:LEU:HD12	1.87	0.56
1:A:542:GLU:OE1	1:A:542:GLU:N	2.24	0.56
1:B:2105:LEU:HD11	1:B:2108:LYS:CB	2.36	0.56
1:A:495:LEU:HD13	1:A:495:LEU:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2320:GLU:O	1:B:2377:LEU:HD11	2.05	0.55
1:B:2418:LYS:HD2	1:B:2423:HIS:NE2	2.21	0.55
1:B:2418:LYS:HD2	1:B:2423:HIS:CD2	2.40	0.55
1:A:122:LEU:HB3	4:A:1079:HOH:O	2.06	0.55
1:A:501:SER:O	1:A:504:ARG:HG2	2.06	0.55
1:B:2014:ARG:HD3	1:B:2018:ARG:HH21	1.71	0.55
1:B:2258:TYR:O	1:B:2259:GLU:HB3	2.06	0.55
1:A:14:ARG:HG2	1:A:60:PRO:HD2	1.88	0.55
1:A:501:SER:HA	1:A:504:ARG:NE	2.18	0.55
1:B:2492:GLN:O	1:B:2496:ARG:HB3	2.06	0.55
1:A:105:LEU:CD2	1:A:108:LYS:H	2.19	0.55
1:A:157:THR:OG1	1:A:253:PRO:HG3	2.06	0.55
1:A:340:PRO:CD	1:A:360:HIS:O	2.51	0.55
1:B:2246:TRP:CH2	1:B:2250:LYS:HG3	2.42	0.55
1:B:2379:HIS:O	1:B:2386:PRO:HA	2.06	0.55
1:B:2405:TRP:CG	1:B:2423:HIS:ND1	2.75	0.55
1:A:57:PRO:O	1:A:72:THR:HG21	2.06	0.55
1:A:105:LEU:HG	4:A:1225:HOH:O	2.06	0.55
1:A:93:GLU:O	1:A:94:VAL:HG23	2.07	0.55
1:B:2004:GLU:OE2	1:B:2007:ARG:NH2	2.37	0.55
1:B:2142:GLY:O	1:B:2143:GLU:HG3	2.06	0.55
1:A:339:THR:HG23	1:A:340:PRO:HD2	1.89	0.55
1:A:479:ASP:HB2	4:A:1159:HOH:O	2.08	0.54
1:A:477:LYS:HB2	1:A:480:LEU:HG	1.89	0.54
1:B:2518:VAL:HG23	1:B:2522:LEU:HB3	1.89	0.54
1:A:570:LEU:O	1:A:574:LEU:HD12	2.07	0.54
1:A:379:HIS:O	1:A:386:PRO:HA	2.08	0.54
1:A:173:GLY:HA3	1:A:225:PHE:HA	1.88	0.54
1:B:2339:THR:HG23	1:B:2340:PRO:HD2	1.89	0.54
1:A:126:LEU:HD23	1:A:128:TYR:OH	2.07	0.54
1:A:152:LEU:O	1:A:158:ILE:HD12	2.08	0.54
1:B:2173:GLY:HA2	1:B:2225:PHE:HA	1.90	0.54
1:B:2327:ASP:OD1	1:B:2328:VAL:N	2.24	0.54
1:B:2497:GLN:HA	1:B:2500:GLU:HG3	1.90	0.54
1:A:53:GLU:HG3	1:A:54:PHE:CD2	2.42	0.54
1:B:2102:GLU:OE1	1:B:2109:ARG:HA	2.07	0.54
1:B:2521:VAL:HG13	1:B:2522:LEU:N	2.22	0.54
1:B:2237:LEU:HD21	1:B:2246:TRP:CD1	2.43	0.53
1:A:235:SER:OG	1:A:237:LEU:HG	2.08	0.53
1:A:271:TYR:O	1:A:274:PHE:HB2	2.09	0.53
1:B:2434:ARG:O	1:B:2438:ILE:HG12	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:532:THR:HG22	1:A:582:GLU:HG2	1.90	0.53
1:A:117:HIS:CD2	1:A:281:LEU:HD11	2.43	0.53
1:A:170:GLU:OE2	1:A:230:LEU:HD23	2.09	0.53
1:A:171:VAL:HG21	1:A:252:PHE:CE1	2.44	0.53
1:B:2328:VAL:HA	1:B:2342:GLY:HA2	1.91	0.53
1:A:556:ARG:HB2	1:A:556:ARG:NH2	2.23	0.53
1:B:2107:ARG:O	1:B:2109:ARG:N	2.41	0.53
1:B:2113:TYR:HD2	1:B:2292:LEU:HA	1.73	0.53
1:B:2298:TRP:O	1:B:2301:LEU:O	2.27	0.53
1:B:2494:LEU:HA	1:B:2497:GLN:HG2	1.91	0.53
1:A:106:GLY:O	1:A:107:ARG:HB2	2.07	0.53
1:B:2009:ARG:NH2	1:B:2043:GLU:OE1	2.42	0.53
1:B:2409:CYS:SG	1:B:2411:GLU:N	2.74	0.53
1:A:69:LEU:O	1:A:150:GLN:HG3	2.09	0.53
1:B:2532:THR:HG22	1:B:2533:MET:N	2.24	0.53
1:A:123:SER:HA	1:A:174:GLU:HG2	1.91	0.53
1:A:297:LEU:O	1:A:301:LEU:HD12	2.09	0.53
1:A:545:LEU:O	1:A:547:VAL:N	2.42	0.53
1:A:57:PRO:HG2	1:A:74:ARG:HD2	1.90	0.53
1:A:558:ILE:O	1:A:562:LEU:HG	2.08	0.52
1:B:2090:THR:O	1:B:2094:VAL:HG23	2.07	0.52
1:B:2103:ARG:O	1:B:2104:ALA:CB	2.56	0.52
1:A:79:PRO:HB2	1:A:170:GLU:OE2	2.09	0.52
1:B:2118:LYS:HD2	3:B:2700:AMP:P	2.50	0.52
1:B:2239:SER:HB3	1:B:2242:GLU:HB2	1.90	0.52
1:A:224:THR:HA	1:A:253:PRO:O	2.10	0.52
1:A:320:GLU:O	1:A:321:LYS:HD2	2.09	0.52
1:B:2106:GLY:O	1:B:2107:ARG:HG2	2.09	0.52
1:A:535:ARG:HH21	1:A:535:ARG:HG3	1.74	0.52
1:A:41:LEU:CD2	1:A:64:VAL:HG11	2.40	0.52
1:B:2407:GLU:HG2	1:B:2415:ARG:NH1	2.25	0.52
1:A:14:ARG:NH1	1:A:14:ARG:HG3	2.25	0.52
1:A:44:LEU:CD1	1:A:60:PRO:HD2	2.39	0.52
1:A:95:LEU:CD1	1:A:109:ARG:HH21	2.23	0.52
1:B:2076:VAL:O	1:B:2144:VAL:HA	2.09	0.52
1:B:2239:SER:HB3	1:B:2242:GLU:CG	2.39	0.52
1:A:113:TYR:CD2	1:A:292:LEU:HA	2.44	0.52
1:B:2008:ARG:HA	1:B:2011:ASN:ND2	2.24	0.52
1:B:2067:ARG:HG3	1:B:2068:PRO:HD2	1.90	0.52
1:B:2105:LEU:HD13	1:B:2108:LYS:HB2	1.92	0.52
1:A:105:LEU:CD2	1:A:106:GLY:N	2.72	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:TYR:HA	1:A:26:VAL:HG23	1.92	0.52
1:A:347:VAL:HG22	1:A:348:PHE:H	1.74	0.52
1:A:388:VAL:O	1:A:388:VAL:HG22	2.10	0.52
1:A:459:ARG:CA	1:A:459:ARG:HE	2.23	0.52
1:B:2095:LEU:HD13	1:B:2109:ARG:HH21	1.75	0.52
1:A:162:LEU:CD2	1:A:169:LEU:HD23	2.40	0.51
1:A:153:LEU:HD11	1:A:160:ARG:HD3	1.93	0.51
1:A:151:ASN:ND2	1:A:208:LEU:O	2.43	0.51
1:A:509:LEU:O	1:A:513:LEU:HD13	2.10	0.51
1:B:2222:ARG:HD3	1:B:2255:GLU:OE1	2.11	0.51
1:B:2043:GLU:O	1:B:2047:LEU:HD13	2.11	0.51
1:B:2057:PRO:HG2	1:B:2074:ARG:NE	2.25	0.51
1:B:2162:LEU:HD21	1:B:2252:PHE:HE2	1.70	0.51
1:A:14:ARG:NH2	1:A:59:SER:HB2	2.26	0.51
1:A:94:VAL:CG1	1:A:94:VAL:O	2.51	0.51
1:B:2440:HIS:O	1:B:2440:HIS:HD2	1.93	0.51
1:A:109:ARG:H	1:A:110:PRO:CD	2.23	0.51
1:A:14:ARG:HE	1:A:59:SER:HB2	1.75	0.51
1:B:2392:LEU:C	1:B:2394:GLU:H	2.13	0.51
1:A:563:LYS:HE2	4:A:1134:HOH:O	2.10	0.51
1:B:2441:TYR:CZ	1:B:2447:MET:HG3	2.46	0.51
1:A:238:LYS:C	1:A:295:LEU:HD22	2.30	0.51
1:B:2095:LEU:HD11	1:B:2109:ARG:NE	2.26	0.51
1:B:2309:ARG:HB2	1:B:2309:ARG:NH1	2.25	0.51
1:A:99:GLU:CA	1:A:102:GLU:HG3	2.34	0.51
1:B:2120:ASP:O	1:B:2121:GLY:C	2.46	0.51
1:A:122:LEU:HD21	1:A:205:ALA:HB2	1.93	0.51
1:B:2102:GLU:HG2	1:B:2105:LEU:HD23	1.93	0.51
1:B:2157:THR:OG1	1:B:2253:PRO:HG3	2.12	0.50
1:A:118:LYS:HG3	1:A:288:VAL:CA	2.41	0.50
1:A:13:LEU:HD11	1:A:43:GLU:HG2	1.92	0.50
1:A:278:ARG:O	1:A:279:HIS:HD2	1.94	0.50
1:A:118:LYS:CG	1:A:289:VAL:HG23	2.39	0.50
1:A:505:GLY:HA3	1:A:584:LYS:HB2	1.92	0.50
1:B:2436:GLU:HA	1:B:2436:GLU:OE1	2.11	0.50
1:B:2487:GLY:O	1:B:2489:LYS:N	2.44	0.50
1:A:254:VAL:HG13	1:A:254:VAL:O	2.11	0.50
1:A:399:GLU:O	1:A:399:GLU:HG2	2.12	0.50
1:A:14:ARG:NE	1:A:59:SER:HB2	2.26	0.50
1:B:2023:ARG:NH1	1:B:2031:GLU:HG3	2.23	0.50
1:B:2109:ARG:NH1	1:B:2109:ARG:HG2	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2171:VAL:HG12	1:B:2225:PHE:HD1	1.77	0.50
1:B:2371:ARG:HB3	1:B:2400:GLU:HB3	1.93	0.50
1:A:27:LEU:O	1:A:28:ALA:HB3	2.11	0.50
1:A:419:GLU:OE1	1:A:424:ARG:HD2	2.12	0.50
1:B:2225:PHE:N	1:B:2225:PHE:CD2	2.79	0.50
1:B:2361:ASN:O	1:B:2361:ASN:OD1	2.29	0.50
1:A:475:LEU:O	1:A:476:ARG:C	2.50	0.50
1:B:2265:GLU:CD	1:B:2265:GLU:H	2.14	0.50
1:B:2501:SER:O	1:B:2503:HIS:N	2.44	0.50
1:A:109:ARG:N	1:A:110:PRO:CD	2.74	0.50
1:A:379:HIS:HD2	4:A:702:HOH:O	1.94	0.50
1:A:450:GLU:HB2	1:A:497:GLN:HE22	1.77	0.50
1:A:473:TYR:O	1:A:476:ARG:HG3	2.11	0.50
1:A:14:ARG:HH21	1:A:59:SER:HB2	1.77	0.50
1:B:2098:GLU:O	1:B:2101:LEU:HB3	2.11	0.50
1:B:2142:GLY:O	1:B:2143:GLU:CG	2.60	0.50
1:B:2396:ARG:HA	1:B:2400:GLU:OE1	2.12	0.50
1:A:129:GLU:C	1:A:131:GLY:N	2.66	0.50
1:A:195:LYS:CD	1:A:367:GLU:HG2	2.42	0.50
1:B:2109:ARG:HG2	1:B:2109:ARG:HH11	1.77	0.50
1:A:542:GLU:CD	1:A:542:GLU:H	2.07	0.49
1:B:2122:LEU:HD11	1:B:2208:LEU:HD23	1.93	0.49
1:B:2063:GLN:O	1:B:2064:VAL:O	2.30	0.49
1:A:111:PHE:HE1	4:A:1225:HOH:O	1.95	0.49
1:A:148:VAL:HG22	1:A:148:VAL:O	2.13	0.49
1:A:185:LEU:HD12	1:A:185:LEU:O	2.11	0.49
1:A:389:LEU:CD1	1:A:390:ARG:HG2	2.42	0.49
1:A:472:LEU:O	1:A:475:LEU:HB2	2.12	0.49
1:A:447:MET:CE	1:A:509:LEU:HD23	2.42	0.49
1:A:108:LYS:HE3	1:A:111:PHE:HE2	1.78	0.49
1:A:430:CYS:HB3	1:A:433:LYS:HD3	1.94	0.49
1:A:459:ARG:NE	1:A:459:ARG:HA	2.28	0.49
1:B:2044:LEU:HD22	1:B:2048:GLU:CD	2.33	0.49
1:A:94:VAL:HA	1:A:97:PHE:HB3	1.94	0.49
1:A:266:GLY:O	1:A:269:GLU:HB3	2.13	0.49
1:A:524:ARG:HB2	1:A:524:ARG:HH11	1.77	0.49
1:A:77:ARG:HG3	4:A:1090:HOH:O	2.13	0.49
1:B:2122:LEU:HD11	1:B:2208:LEU:CB	2.43	0.49
1:B:2495:LEU:HD23	1:B:2495:LEU:O	2.13	0.49
1:A:433:LYS:NZ	1:A:433:LYS:CB	2.76	0.49
1:B:2195:LYS:HE3	1:B:2364:TYR:HD1	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2451:GLY:HA3	1:B:2497:GLN:NE2	2.28	0.49
1:A:22:TYR:HA	1:A:26:VAL:CG2	2.42	0.49
1:B:2411:GLU:HG2	1:B:2432:ALA:HB2	1.95	0.49
1:B:2533:MET:HG2	1:B:2571:VAL:HG21	1.95	0.49
1:A:105:LEU:CD2	1:A:108:LYS:HG2	2.42	0.49
1:B:2113:TYR:O	1:B:2260:LYS:HA	2.13	0.48
1:B:2397:THR:HG23	1:B:2399:GLU:H	1.78	0.48
1:B:2533:MET:CE	1:B:2571:VAL:HG21	2.43	0.48
1:A:531:GLY:O	1:A:582:GLU:HA	2.13	0.48
1:B:2222:ARG:NH2	1:B:2255:GLU:OE2	2.46	0.48
1:B:2424:ARG:CB	1:B:2424:ARG:HH21	2.26	0.48
1:A:122:LEU:CD2	4:A:1079:HOH:O	2.62	0.48
1:B:2047:LEU:N	1:B:2047:LEU:HD12	2.28	0.48
1:B:2196:VAL:HG21	1:B:2360:HIS:HD2	1.75	0.48
1:A:191:GLU:CD	1:A:337:ARG:HE	2.16	0.48
1:A:332:VAL:HG11	1:A:411:GLU:HG3	1.95	0.48
1:B:2057:PRO:HA	1:B:2062:GLU:CG	2.35	0.48
1:B:2126:LEU:HD22	1:B:2225:PHE:CE1	2.48	0.48
1:B:2414:HIS:ND1	1:B:2415:ARG:N	2.60	0.48
1:B:2515:LEU:HB2	1:B:2518:VAL:CG1	2.43	0.48
1:A:153:LEU:CD1	1:A:160:ARG:HD3	2.43	0.48
1:A:162:LEU:HD23	1:A:169:LEU:HD23	1.96	0.48
1:A:295:LEU:O	1:A:298:TRP:HB2	2.14	0.48
1:A:44:LEU:HD13	1:A:61:THR:HG23	1.95	0.48
1:B:2023:ARG:O	1:B:2028:ALA:N	2.46	0.48
1:B:2333:GLY:O	1:B:2335:THR:N	2.46	0.48
1:B:2553:LEU:HD12	1:B:2553:LEU:H	1.78	0.48
1:A:560:GLU:HA	1:A:560:GLU:OE2	2.13	0.48
1:A:56:SER:O	1:A:58:ASP:N	2.45	0.48
1:A:14:ARG:NE	1:A:59:SER:CB	2.77	0.48
1:A:19:TYR:O	1:A:22:TYR:HB3	2.13	0.48
1:A:392:LEU:HD23	1:A:395:ARG:NH1	2.29	0.48
1:B:2470:ALA:HB2	1:B:2574:LEU:HD23	1.95	0.48
1:A:72:THR:O	1:A:147:GLU:HB3	2.13	0.48
1:A:181:ALA:O	1:A:182:PHE:C	2.52	0.48
1:A:246:TRP:CZ2	1:A:250:LYS:HE3	2.49	0.48
1:A:466:VAL:HG12	1:A:467:ARG:N	2.28	0.48
1:A:473:TYR:CD1	1:A:473:TYR:N	2.81	0.48
1:B:2121:GLY:HA2	1:B:2174:GLU:OE2	2.13	0.48
1:A:357:VAL:CG2	1:A:387:GLU:HA	2.44	0.48
1:B:2088:ALA:HA	1:B:2093:GLU:OE2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:LEU:N	1:A:281:LEU:HD23	2.29	0.48
1:B:2195:LYS:HE3	1:B:2364:TYR:CE1	2.49	0.48
1:B:2473:TYR:N	1:B:2473:TYR:CD1	2.82	0.48
1:A:191:GLU:OE1	1:A:335:THR:HG21	2.14	0.47
1:A:459:ARG:NH1	1:A:462:GLU:HB3	2.25	0.47
1:A:468:ASP:OD2	1:A:468:ASP:C	2.53	0.47
1:A:494:LEU:HD23	1:A:494:LEU:C	2.34	0.47
1:A:552:GLU:HG2	1:A:556:ARG:HH22	1.78	0.47
1:B:2007:ARG:HH22	1:B:2130:GLU:CD	2.16	0.47
1:B:2424:ARG:HH21	1:B:2424:ARG:HB2	1.79	0.47
1:A:263:GLY:O	1:A:264:ALA:C	2.52	0.47
1:A:545:LEU:C	1:A:547:VAL:H	2.18	0.47
1:A:537:LEU:CD2	1:A:568:ARG:HE	2.10	0.47
1:B:2484:GLU:O	1:B:2485:ARG:HB2	2.15	0.47
1:A:166:PRO:HG2	1:A:234:GLU:HB3	1.87	0.47
1:A:162:LEU:HD21	1:A:252:PHE:HZ	1.79	0.47
1:A:129:GLU:C	1:A:131:GLY:H	2.18	0.47
1:A:405:TRP:CD1	1:A:423:HIS:HB2	2.49	0.47
1:A:93:GLU:O	1:A:94:VAL:CG2	2.63	0.47
1:B:2349:ILE:O	1:B:2350:GLU:HB2	2.13	0.47
1:B:2427:ASN:ND2	1:B:2429:LEU:H	2.12	0.47
1:B:2515:LEU:HB2	1:B:2518:VAL:HG11	1.96	0.47
1:A:292:LEU:HB2	1:A:310:PHE:O	2.15	0.47
1:B:2398:GLY:C	1:B:2400:GLU:H	2.17	0.47
1:B:2548:GLU:O	1:B:2549:GLU:HB2	2.14	0.47
1:B:2572:ARG:O	1:B:2575:LYS:HB3	2.15	0.47
1:B:2564:ASP:OD2	1:B:2566:ALA:N	2.47	0.47
1:B:2539:ALA:HA	1:B:2543:GLU:OE2	2.14	0.47
1:A:15:ASP:OD2	1:A:161:ARG:NH1	2.43	0.47
1:A:186:ASN:O	1:A:190:GLU:HG3	2.14	0.47
1:A:81:ARG:NH2	1:A:306:ARG:HG2	2.29	0.47
1:B:2019:TYR:O	1:B:2022:TYR:HB3	2.15	0.47
1:A:105:LEU:HD21	1:A:108:LYS:H	1.79	0.47
1:A:435:PHE:CZ	1:A:454:GLU:HG3	2.50	0.47
1:A:71:PRO:HG3	1:A:151:ASN:OD1	2.15	0.47
1:B:2553:LEU:HD12	1:B:2553:LEU:N	2.30	0.47
1:A:222:ARG:HH11	1:A:222:ARG:HG3	1.78	0.46
1:B:2373:GLY:C	1:B:2400:GLU:HG2	2.36	0.46
1:B:2447:MET:HG2	1:B:2512:ALA:CB	2.45	0.46
1:A:126:LEU:HD21	1:A:158:ILE:CG2	2.45	0.46
1:A:166:PRO:HB3	1:A:234:GLU:CD	2.35	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2098:GLU:OE2	1:B:2263:GLY:HA2	2.15	0.46
1:B:2246:TRP:CZ2	1:B:2250:LYS:HE3	2.50	0.46
1:B:2323:THR:OG1	1:B:2345:GLU:HB3	2.14	0.46
1:A:129:GLU:O	1:A:131:GLY:N	2.48	0.46
1:A:287:GLY:HA3	1:A:315:LYS:HA	1.97	0.46
1:A:365:ILE:HD13	1:A:403:ILE:HG21	1.98	0.46
1:A:521:VAL:HG13	1:A:522:LEU:N	2.30	0.46
1:B:2150:GLN:NE2	1:B:2150:GLN:CA	2.79	0.46
1:B:2376:VAL:HG12	1:B:2391:VAL:CA	2.43	0.46
1:B:2151:ASN:OD1	1:B:2208:LEU:O	2.34	0.46
1:B:2474:HIS:C	1:B:2476:ARG:H	2.18	0.46
1:A:515:LEU:HB2	1:A:518:VAL:HG12	1.95	0.46
1:B:2002:THR:HG22	1:B:2005:GLU:HG3	1.98	0.46
1:B:2045:LYS:O	1:B:2049:GLU:HB2	2.16	0.46
1:A:102:GLU:O	1:A:104:ALA:N	2.49	0.46
1:A:122:LEU:HD22	4:A:1079:HOH:O	2.14	0.46
1:A:39:ARG:NE	1:A:39:ARG:HA	2.29	0.46
1:A:506:LEU:HD13	1:A:527:ALA:HA	1.97	0.46
1:B:2374:ASP:CG	1:B:2391:VAL:HG21	2.36	0.46
1:A:295:LEU:HA	1:A:298:TRP:CD1	2.51	0.46
1:A:98:GLU:OE2	1:A:109:ARG:O	2.34	0.46
1:B:2072:THR:OG1	1:B:2072:THR:O	2.31	0.46
1:A:166:PRO:CB	1:A:234:GLU:HB3	2.44	0.46
1:A:323:THR:OG1	1:A:345:GLU:HB3	2.16	0.46
1:A:431:PRO:HG3	1:A:434:ARG:HH11	1.81	0.46
1:B:2063:GLN:O	1:B:2064:VAL:C	2.54	0.46
1:B:2157:THR:O	1:B:2253:PRO:HD3	2.16	0.46
1:B:2073:PHE:CE2	1:B:2209:ARG:HA	2.51	0.46
1:B:2170:GLU:HB3	1:B:2230:LEU:H	1.80	0.46
1:A:121:GLY:O	1:A:201:ARG:HG3	2.16	0.45
1:B:2244:LEU:O	1:B:2247:LEU:HB2	2.16	0.45
1:B:2115:VAL:HG21	1:B:2267:VAL:HG12	1.98	0.45
1:A:116:GLU:HB3	1:A:258:TYR:HB3	1.97	0.45
1:A:475:LEU:O	1:A:477:LYS:N	2.49	0.45
1:B:2015:ASP:OD1	1:B:2160:ARG:HD2	2.15	0.45
1:A:185:LEU:HD11	1:A:189:LEU:HD11	1.98	0.45
1:A:535:ARG:NH2	1:A:535:ARG:HG3	2.32	0.45
1:A:56:SER:C	1:A:58:ASP:N	2.69	0.45
1:A:195:LYS:HD2	1:A:367:GLU:CG	2.46	0.45
1:B:2116:GLU:OE2	1:B:2256:HIS:NE2	2.42	0.45
1:B:2546:GLU:HB2	4:B:1226:HOH:O	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:ASN:HB3	1:A:208:LEU:HD12	1.99	0.45
1:A:86:ASP:O	1:A:312:LEU:HD12	2.17	0.45
1:A:90:THR:OG1	1:A:92:GLU:HG2	2.16	0.45
1:B:2303:TYR:CD2	1:B:2308:PRO:HB3	2.52	0.45
1:B:2496:ARG:HH11	1:B:2496:ARG:CG	2.30	0.45
1:A:14:ARG:O	1:A:18:ARG:HG3	2.16	0.45
1:B:2125:ASN:ND2	1:B:2172:ARG:CD	2.80	0.45
1:B:2239:SER:O	1:B:2243:LEU:N	2.47	0.45
1:B:2496:ARG:HD2	1:B:2496:ARG:O	2.17	0.45
1:B:2540:SER:O	1:B:2541:LEU:C	2.55	0.45
1:A:548:GLU:O	1:A:549:GLU:CB	2.64	0.44
1:B:2128:TYR:HA	1:B:2132:VAL:O	2.17	0.44
1:B:2277:GLN:O	1:B:2278:ARG:C	2.54	0.44
1:B:2476:ARG:O	1:B:2495:LEU:HD11	2.17	0.44
1:A:91:TYR:OH	1:A:265:GLU:HG3	2.17	0.44
1:B:2138:THR:O	1:B:2145:GLY:HA3	2.16	0.44
1:B:2142:GLY:C	1:B:2143:GLU:HG3	2.38	0.44
1:A:237:LEU:HD13	1:A:243:LEU:HD12	1.98	0.44
1:A:436:GLU:HA	1:A:436:GLU:OE2	2.16	0.44
1:A:518:VAL:O	1:A:518:VAL:CG1	2.65	0.44
1:B:2071:PRO:HG2	1:B:2073:PHE:CE1	2.52	0.44
1:B:2073:PHE:HE2	1:B:2209:ARG:HA	1.82	0.44
1:B:2095:LEU:CD1	1:B:2109:ARG:HH21	2.31	0.44
1:B:2224:THR:O	1:B:2224:THR:CG2	2.65	0.44
1:B:2332:VAL:HG21	1:B:2411:GLU:HB2	1.98	0.44
1:B:2440:HIS:O	1:B:2440:HIS:CD2	2.71	0.44
1:B:2105:LEU:C	1:B:2105:LEU:HD12	2.37	0.44
1:A:44:LEU:O	1:A:48:GLU:HG3	2.18	0.44
1:B:2171:VAL:HG12	1:B:2225:PHE:CD1	2.52	0.44
1:B:2170:GLU:HB3	1:B:2230:LEU:N	2.32	0.44
1:B:2494:LEU:O	1:B:2497:GLN:HG2	2.17	0.44
1:A:122:LEU:N	1:A:122:LEU:HD12	2.33	0.44
1:A:169:LEU:HA	1:A:230:LEU:O	2.18	0.44
1:A:61:THR:HA	1:A:64:VAL:CG1	2.47	0.44
1:B:2414:HIS:HD1	1:B:2415:ARG:N	2.14	0.44
1:A:545:LEU:CD2	1:A:552:GLU:HA	2.48	0.44
1:B:2014:ARG:HD3	1:B:2018:ARG:NH2	2.31	0.44
1:B:2105:LEU:CD1	1:B:2108:LYS:HD3	2.48	0.44
1:B:2118:LYS:O	1:B:2285:ALA:HA	2.18	0.44
1:B:2233:GLU:HG3	1:B:2234:GLU:H	1.83	0.44
1:B:2404:ARG:CB	1:B:2404:ARG:HH21	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2552:GLU:O	1:B:2555:ALA:HB3	2.18	0.44
1:A:108:LYS:HE3	1:A:111:PHE:CE2	2.53	0.43
1:A:81:ARG:HH21	1:A:306:ARG:HG2	1.82	0.43
1:B:2392:LEU:C	1:B:2394:GLU:N	2.71	0.43
1:B:2469:VAL:HG22	1:B:2570:LEU:HD11	1.99	0.43
1:A:97:PHE:CG	1:A:312:LEU:HD22	2.53	0.43
1:B:2101:LEU:C	1:B:2103:ARG:H	2.21	0.43
1:B:2452:LEU:HG	1:B:2457:ILE:CG1	2.48	0.43
1:A:10:ILE:HD12	1:A:54:PHE:CD1	2.50	0.43
1:A:162:LEU:HD21	1:A:252:PHE:CZ	2.54	0.43
1:A:415:ARG:HH11	1:A:415:ARG:HG3	1.82	0.43
1:A:457:ILE:O	1:A:461:LEU:HB2	2.19	0.43
1:A:456:LEU:O	1:A:460:LEU:HG	2.19	0.43
1:B:2044:LEU:HD22	1:B:2048:GLU:HG3	2.01	0.43
1:B:2080:THR:HG23	1:B:2230:LEU:HD23	1.99	0.43
1:B:2259:GLU:CD	1:B:2273:ARG:HH22	2.22	0.43
1:B:2359:LEU:HD22	1:B:2370:ILE:CD1	2.49	0.43
1:B:2332:VAL:HG23	1:B:2432:ALA:CB	2.48	0.43
1:B:2499:GLU:O	1:B:2499:GLU:HG3	2.16	0.43
1:B:2088:ALA:HB1	1:B:2093:GLU:HB2	2.01	0.43
1:B:2095:LEU:HD11	1:B:2109:ARG:HE	1.82	0.43
1:B:2359:LEU:O	1:B:2360:HIS:C	2.57	0.43
1:A:466:VAL:CG1	1:A:467:ARG:N	2.81	0.43
1:A:506:LEU:O	1:A:506:LEU:HD22	2.18	0.43
1:B:2157:THR:HB	1:B:2253:PRO:CB	2.48	0.43
1:B:2478:GLU:HG3	1:B:2495:LEU:CD1	2.38	0.43
1:A:231:GLY:O	1:A:234:GLU:HB2	2.19	0.43
1:B:2425:CYS:SG	1:B:2427:ASN:HB3	2.59	0.43
1:A:105:LEU:HD22	1:A:108:LYS:H	1.83	0.43
1:B:2102:GLU:HG2	1:B:2105:LEU:CD2	2.48	0.43
1:A:16:LEU:H	1:A:16:LEU:CD1	2.32	0.43
1:A:342:GLY:N	1:A:357:VAL:O	2.48	0.43
1:A:371:ARG:HD3	1:A:396:ARG:CZ	2.49	0.43
1:A:496:ARG:O	1:A:500:GLU:HG3	2.19	0.43
1:B:2233:GLU:CG	1:B:2234:GLU:H	2.32	0.43
1:B:2361:ASN:O	1:B:2364:TYR:N	2.51	0.43
1:A:368:LEU:O	1:A:369:ASP:C	2.56	0.42
1:A:477:LYS:HB2	1:A:480:LEU:CD1	2.49	0.42
1:A:507:GLU:HG2	1:A:524:ARG:HG3	2.01	0.42
1:A:575:LYS:C	1:A:577:ALA:H	2.22	0.42
1:A:211:LYS:HB2	1:A:211:LYS:NZ	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:ILE:C	1:A:374:ASP:N	2.72	0.42
1:A:72:THR:C	1:A:74:ARG:H	2.22	0.42
1:B:2089:PHE:CD1	1:B:2089:PHE:N	2.87	0.42
1:B:2113:TYR:CD2	1:B:2292:LEU:HA	2.52	0.42
1:A:238:LYS:O	1:A:295:LEU:HB2	2.18	0.42
1:B:2017:ILE:HD12	1:B:2044:LEU:HD12	2.01	0.42
1:B:2087:ASN:HD22	1:B:2315:LYS:HD2	1.84	0.42
1:B:2478:GLU:OE2	1:B:2478:GLU:N	2.40	0.42
1:B:2518:VAL:CG1	1:B:2518:VAL:O	2.67	0.42
1:A:389:LEU:HD12	1:A:390:ARG:HG2	2.00	0.42
1:A:51:PHE:N	1:A:52:PRO:HD3	2.34	0.42
1:B:2096:ALA:O	1:B:2100:ARG:HD3	2.19	0.42
1:B:2111:PHE:O	1:B:2262:LEU:HD12	2.19	0.42
1:B:2533:MET:HG2	1:B:2571:VAL:CG2	2.50	0.42
1:A:515:LEU:O	1:A:518:VAL:HG12	2.19	0.42
1:B:2392:LEU:HB3	1:B:2394:GLU:HG2	2.01	0.42
1:A:118:LYS:HG2	1:A:289:VAL:CG2	2.46	0.42
1:A:150:GLN:O	1:A:153:LEU:HB2	2.20	0.42
1:A:36:GLU:O	1:A:39:ARG:HB2	2.20	0.42
1:A:237:LEU:HD13	1:A:243:LEU:HA	2.01	0.42
1:A:362:GLU:CD	1:A:362:GLU:H	2.23	0.42
1:A:368:LEU:HD12	1:A:390:ARG:HA	2.02	0.42
1:A:52:PRO:O	1:A:55:LYS:HG3	2.20	0.42
1:A:545:LEU:C	1:A:547:VAL:N	2.73	0.42
1:B:2150:GLN:NE2	1:B:2150:GLN:HA	2.34	0.42
1:B:2115:VAL:CG2	1:B:2267:VAL:HG12	2.50	0.42
1:B:2282:PRO:HG2	1:B:2283:PHE:CD1	2.55	0.42
1:B:2463:LYS:HD3	1:B:2484:GLU:OE2	2.19	0.42
1:A:389:LEU:C	1:A:389:LEU:HD13	2.40	0.42
1:A:427:ASN:C	1:A:427:ASN:HD22	2.22	0.42
1:A:77:ARG:HA	1:A:143:GLU:O	2.20	0.42
1:B:2095:LEU:CD1	1:B:2109:ARG:HE	2.32	0.42
1:B:2496:ARG:O	1:B:2500:GLU:HG3	2.19	0.42
1:A:374:ASP:OD2	1:A:400:GLU:HG2	2.19	0.41
1:A:584:LYS:HG2	1:A:584:LYS:OXT	2.20	0.41
1:B:2002:THR:CG2	1:B:2005:GLU:H	2.30	0.41
1:B:2057:PRO:C	1:B:2062:GLU:HG3	2.41	0.41
1:B:2065:GLY:C	1:B:2067:ARG:N	2.72	0.41
1:B:2390:ARG:NH1	1:B:2392:LEU:CD2	2.83	0.41
1:B:2332:VAL:HG21	1:B:2411:GLU:CB	2.50	0.41
1:A:24:TYR:O	1:A:26:VAL:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:ARG:HD2	1:A:316:PHE:CD2	2.55	0.41
1:B:2239:SER:HB3	1:B:2242:GLU:CB	2.50	0.41
1:B:2278:ARG:O	1:B:2280:ALA:N	2.53	0.41
1:A:274:PHE:C	1:A:276:ALA:N	2.74	0.41
1:A:2:THR:O	1:A:5:GLU:N	2.53	0.41
1:A:456:LEU:HG	1:A:460:LEU:HD11	2.03	0.41
1:A:568:ARG:HA	1:A:568:ARG:HD3	1.75	0.41
1:B:2475:LEU:O	1:B:2476:ARG:C	2.58	0.41
1:A:274:PHE:O	1:A:276:ALA:N	2.53	0.41
1:B:2174:GLU:HG3	1:B:2226:TYR:CE1	2.56	0.41
1:B:2345:GLU:O	1:B:2346:PRO:C	2.59	0.41
1:A:161:ARG:HG2	1:A:161:ARG:HH11	1.85	0.41
1:A:441:TYR:CD1	1:A:512:ALA:HB1	2.55	0.41
1:B:2303:TYR:HA	1:B:2308:PRO:HA	2.03	0.41
1:B:2330:PHE:HE1	1:B:2405:TRP:CD2	2.38	0.41
1:B:2359:LEU:HD22	1:B:2370:ILE:HD13	2.01	0.41
1:B:2379:HIS:CG	1:B:2380:LYS:N	2.87	0.41
1:B:2424:ARG:CB	1:B:2424:ARG:NH2	2.84	0.41
1:B:2487:GLY:C	1:B:2489:LYS:N	2.73	0.41
1:A:427:ASN:HA	1:A:428:PRO:HD3	1.91	0.41
1:B:2098:GLU:OE1	1:B:2264:ALA:N	2.53	0.41
1:B:2226:TYR:CD2	1:B:2226:TYR:C	2.93	0.41
1:B:2438:ILE:O	1:B:2441:TYR:N	2.51	0.41
1:A:294:ASP:OD1	1:A:297:LEU:HB2	2.20	0.41
1:B:2278:ARG:C	1:B:2280:ALA:H	2.23	0.41
1:A:221:LEU:H	1:A:221:LEU:CD1	2.34	0.41
1:A:80:THR:CG2	1:A:230:LEU:HD22	2.41	0.41
1:A:374:ASP:OD2	1:A:396:ARG:HG2	2.20	0.41
1:B:2007:ARG:HB2	1:B:2054:PHE:CZ	2.56	0.41
1:B:2221:LEU:HD12	1:B:2221:LEU:HA	1.90	0.41
1:B:2360:HIS:CE1	1:B:2387:GLU:OE1	2.74	0.41
1:B:2506:LEU:HB2	1:B:2583:SER:HA	2.02	0.41
1:B:2521:VAL:HG13	1:B:2522:LEU:H	1.86	0.41
1:A:358:THR:HG23	1:A:359:LEU:O	2.21	0.41
1:B:2098:GLU:O	1:B:2102:GLU:HG3	2.21	0.41
1:B:2330:PHE:HE1	1:B:2405:TRP:CE2	2.39	0.41
1:A:20:HIS:CD2	1:A:32:ILE:HG12	2.55	0.41
1:A:433:LYS:HB3	1:A:433:LYS:NZ	2.36	0.41
1:A:518:VAL:HA	1:A:522:LEU:HD12	2.02	0.41
1:A:73:PHE:CD2	1:A:73:PHE:N	2.87	0.41
1:B:2434:ARG:HG2	1:B:2467:ARG:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2442:ALA:O	1:B:2443:SER:O	2.38	0.41
1:A:120:ASP:C	1:A:120:ASP:OD1	2.59	0.41
1:A:497:GLN:C	1:A:499:GLU:N	2.75	0.41
1:A:530:PHE:O	1:A:532:THR:N	2.48	0.41
1:A:532:THR:HA	1:A:581:MET:O	2.21	0.41
1:A:166:PRO:HG2	1:A:234:GLU:CB	2.48	0.40
1:A:195:LYS:NZ	4:A:1096:HOH:O	2.54	0.40
1:B:2012:GLU:O	1:B:2016:LEU:HG	2.20	0.40
1:B:2025:TYR:N	1:B:2025:TYR:CD1	2.90	0.40
1:B:2122:LEU:HD23	1:B:2122:LEU:HA	1.66	0.40
1:B:2265:GLU:HB3	4:B:1209:HOH:O	2.20	0.40
1:B:2501:SER:C	1:B:2503:HIS:N	2.74	0.40
1:A:14:ARG:CZ	1:A:59:SER:HB2	2.51	0.40
1:A:339:THR:HG22	1:A:340:PRO:N	2.36	0.40
1:A:72:THR:OG1	1:A:72:THR:O	2.39	0.40
1:B:2049:GLU:HA	1:B:2049:GLU:OE1	2.21	0.40
1:B:2074:ARG:HH12	1:B:2076:VAL:HG22	1.78	0.40
1:B:2102:GLU:CB	1:B:2105:LEU:HD23	2.51	0.40
1:B:2412:CYS:HB3	1:B:2430:CYS:SG	2.61	0.40
1:B:2424:ARG:HB3	1:B:2424:ARG:NH2	2.36	0.40
1:B:2424:ARG:O	1:B:2424:ARG:HG3	2.22	0.40
1:B:2506:LEU:HG	1:B:2581:MET:O	2.21	0.40
1:A:109:ARG:O	1:A:111:PHE:N	2.55	0.40
1:A:278:ARG:NH1	1:A:316:PHE:CB	2.80	0.40
1:A:394:GLU:OE2	1:A:394:GLU:N	2.53	0.40
1:A:429:LEU:O	1:A:430:CYS:C	2.58	0.40
1:A:452:LEU:HD22	1:A:494:LEU:HD11	2.03	0.40
1:A:58:ASP:OD2	1:A:74:ARG:NE	2.48	0.40
1:A:92:GLU:O	1:A:95:LEU:HB3	2.22	0.40
1:B:2405:TRP:HB2	1:B:2423:HIS:HD1	1.85	0.40
1:B:2427:ASN:HD22	1:B:2428:PRO:CD	2.34	0.40
1:A:7:ARG:NH1	1:A:129:GLU:OE1	2.52	0.40
1:A:275:LEU:HD12	1:A:275:LEU:O	2.21	0.40
1:A:319:GLU:HG3	1:A:349:ILE:CG2	2.46	0.40
1:A:545:LEU:HD21	1:A:552:GLU:HA	2.02	0.40
1:B:2008:ARG:HG3	1:B:2130:GLU:HG3	2.03	0.40
1:B:2027:LEU:O	1:B:2028:ALA:HB3	2.22	0.40
1:B:2496:ARG:HD2	1:B:2496:ARG:C	2.42	0.40
1:A:347:VAL:HG13	1:A:348:PHE:N	2.36	0.40
1:B:2166:PRO:HG3	1:B:2234:GLU:HG2	2.02	0.40
1:B:2493:ASN:O	1:B:2496:ARG:HG3	2.21	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	582/584 (100%)	478 (82%)	71 (12%)	33 (6%)	1	5
1	B	582/584 (100%)	463 (80%)	88 (15%)	31 (5%)	2	6
All	All	1164/1168 (100%)	941 (81%)	159 (14%)	64 (6%)	2	5

All (64) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	62	GLU
1	A	64	VAL
1	A	94	VAL
1	A	104	ALA
1	A	109	ARG
1	A	234	GLU
1	A	448	ASP
1	B	2064	VAL
1	B	2104	ALA
1	B	2194	GLU
1	B	2328	VAL
1	B	2360	HIS
1	B	2361	ASN
1	B	2362	GLU
1	B	2402	PRO
1	B	2443	SER
1	B	2446	ALA
1	A	25	TYR
1	A	103	ARG
1	A	221	LEU
1	A	263	GLY
1	A	373	GLY

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Mol	Chain	Res	Type
1	A	452	LEU
1	A	518	VAL
1	A	546	GLU
1	B	2108	LYS
1	B	2279	HIS
1	B	2334	ARG
1	B	2476	ARG
1	B	2488	GLU
1	B	2502	LYS
1	B	2531	GLY
1	A	106	GLY
1	A	275	LEU
1	A	412	CYS
1	A	476	ARG
1	A	514	GLY
1	B	2120	ASP
1	B	2143	GLU
1	B	2233	GLU
1	B	2304	THR
1	B	2346	PRO
1	A	73	PHE
1	A	105	LEU
1	A	477	LYS
1	A	483	LEU
1	A	576	GLU
1	B	2030	PRO
1	B	2364	TYR
1	B	2399	GLU
1	B	2552	GLU
1	A	3	ARG
1	A	130	GLU
1	A	516	PRO
1	B	2123	SER
1	B	2259	GLU
1	A	57	PRO
1	B	2341	VAL
1	B	2384	VAL
1	A	148	VAL
1	A	531	GLY
1	A	71	PRO
1	A	384	VAL
1	B	2236	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	499/499 (100%)	469 (94%)	30 (6%)	19	49
1	B	499/499 (100%)	461 (92%)	38 (8%)	13	36
All	All	998/998 (100%)	930 (93%)	68 (7%)	16	42

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	ARG
1	A	41	LEU
1	A	44	LEU
1	A	49	GLU
1	A	95	LEU
1	A	99	GLU
1	A	105	LEU
1	A	107	ARG
1	A	172	ARG
1	A	222	ARG
1	A	234	GLU
1	A	243	LEU
1	A	295	LEU
1	A	314	TYR
1	A	319	GLU
1	A	334	ARG
1	A	347	VAL
1	A	367	GLU
1	A	368	LEU
1	A	371	ARG
1	A	384	VAL
1	A	388	VAL
1	A	427	ASN
1	A	430	CYS
1	A	433	LYS
1	A	444	ARG
1	A	461	LEU

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Mol	Chain	Res	Type
1	A	475	LEU
1	A	495	LEU
1	A	506	LEU
1	B	2013	LEU
1	B	2044	LEU
1	B	2049	GLU
1	B	2092	GLU
1	B	2105	LEU
1	B	2117	HIS
1	B	2122	LEU
1	B	2150	GLN
1	B	2153	LEU
1	B	2162	LEU
1	B	2172	ARG
1	B	2214	ARG
1	B	2226	TYR
1	B	2230	LEU
1	B	2233	GLU
1	B	2240	GLN
1	B	2254	VAL
1	B	2255	GLU
1	B	2269	GLU
1	B	2278	ARG
1	B	2314	TYR
1	B	2360	HIS
1	B	2379	HIS
1	B	2389	LEU
1	B	2405	TRP
1	B	2409	CYS
1	B	2424	ARG
1	B	2427	ASN
1	B	2443	SER
1	B	2479	ASP
1	B	2496	ARG
1	B	2498	ILE
1	B	2499	GLU
1	B	2506	LEU
1	B	2507	GLU
1	B	2513	LEU
1	B	2522	LEU
1	B	2533	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	GLN
1	A	87	ASN
1	A	202	ASN
1	A	240	GLN
1	A	279	HIS
1	A	331	GLN
1	A	379	HIS
1	A	427	ASN
1	A	525	ASN
1	B	2011	ASN
1	B	2087	ASN
1	B	2125	ASN
1	B	2150	GLN
1	B	2151	ASN
1	B	2202	ASN
1	B	2210	GLN
1	B	2277	GLN
1	B	2427	ASN
1	B	2497	GLN
1	B	2503	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	AMP	B	2700	-	18,24,25	1.26	3 (16%)	18,35,38	1.95	4 (22%)
3	AMP	A	700	-	18,24,25	1.20	3 (16%)	18,35,38	1.89	4 (22%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	AMP	B	2700	-	-	1/3/25/26	0/3/3/3
3	AMP	A	700	-	-	1/3/25/26	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2700	AMP	O4'-C1'	2.66	1.44	1.41
3	A	700	AMP	C5-N7	-2.49	1.30	1.39
3	B	2700	AMP	C5-N7	-2.46	1.30	1.39
3	A	700	AMP	C2-N3	2.43	1.36	1.32
3	B	2700	AMP	C2-N3	2.19	1.35	1.32
3	A	700	AMP	O4'-C1'	2.18	1.44	1.41

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2700	AMP	N3-C2-N1	-6.46	118.58	128.68
3	A	700	AMP	N3-C2-N1	-6.20	118.99	128.68
3	A	700	AMP	C3'-C2'-C1'	2.90	105.34	100.98
3	B	2700	AMP	C3'-C2'-C1'	2.78	105.17	100.98
3	B	2700	AMP	C2'-C3'-C4'	2.31	107.14	102.64
3	A	700	AMP	C2'-C3'-C4'	2.27	107.05	102.64
3	A	700	AMP	C4-C5-N7	-2.17	107.14	109.40
3	B	2700	AMP	C4-C5-N7	-2.06	107.25	109.40

There are no chirality outliers.

All (2) torsion outliers are listed below:

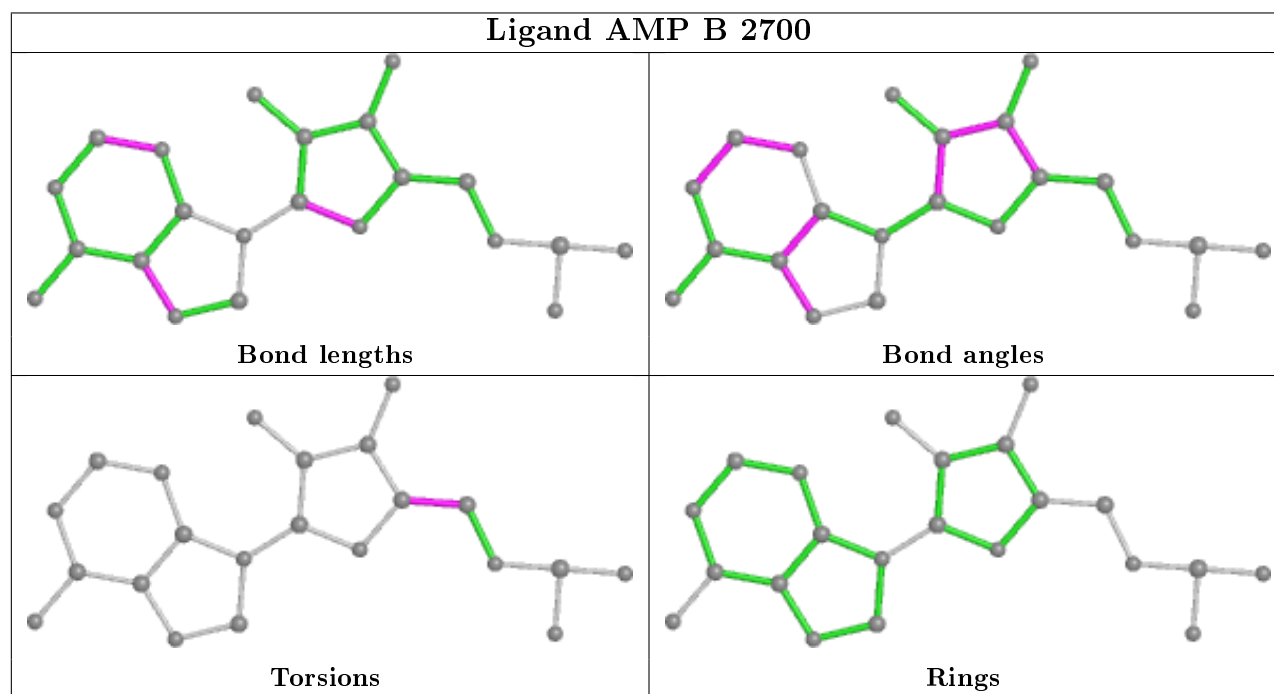
Mol	Chain	Res	Type	Atoms
3	A	700	AMP	O4'-C4'-C5'-O5'
3	B	2700	AMP	O4'-C4'-C5'-O5'

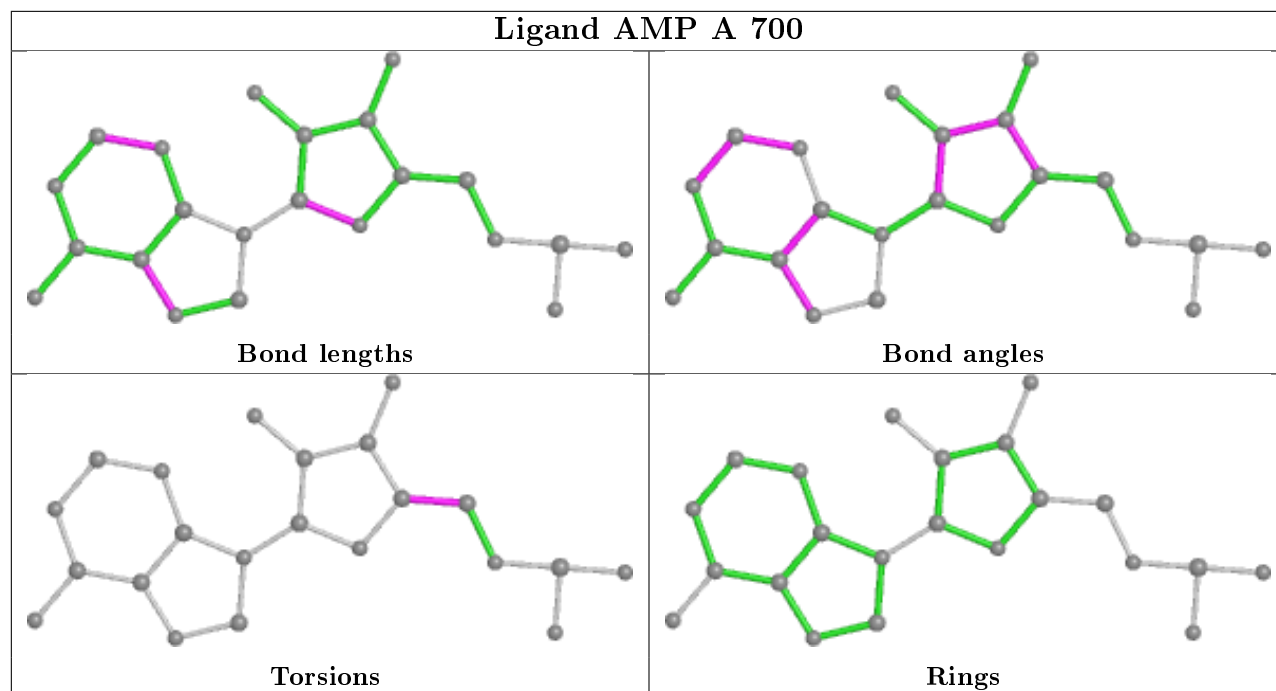
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	2700	AMP	1	0
3	A	700	AMP	2	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	584/584 (100%)	-0.12	15 (2%) 56 52	12, 46, 92, 142	0
1	B	584/584 (100%)	-0.05	18 (3%) 49 44	12, 50, 98, 151	0
All	All	1168/1168 (100%)	-0.08	33 (2%) 53 49	12, 48, 95, 151	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	106	GLY	8.4
1	A	107	ARG	7.3
1	B	2107	ARG	5.6
1	B	2351	GLY	5.5
1	B	2305	ALA	4.8
1	A	487	GLY	3.8
1	A	65	GLY	3.6
1	A	64	VAL	3.4
1	B	2306	ARG	3.3
1	A	397	THR	3.2
1	A	108	LYS	3.0
1	B	2399	GLU	2.9
1	B	2304	THR	2.9
1	B	2106	GLY	2.8
1	A	488	GLU	2.8
1	A	305	ALA	2.6
1	B	2383	GLY	2.5
1	A	584	LYS	2.5
1	B	2234	GLU	2.5
1	B	2484	GLU	2.5
1	A	67	ARG	2.4
1	A	3	ARG	2.3
1	B	2108	LYS	2.3
1	B	2110	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	2444	ARG	2.2
1	B	2476	ARG	2.2
1	A	306	ARG	2.2
1	B	2121	GLY	2.2
1	B	2236	GLY	2.2
1	A	33	SER	2.2
1	B	2485	ARG	2.2
1	A	66	ALA	2.1
1	B	2035	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

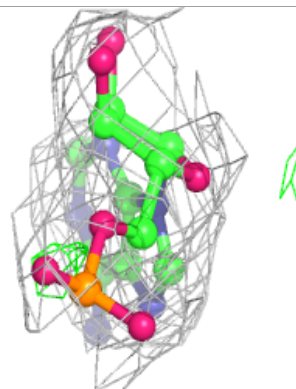
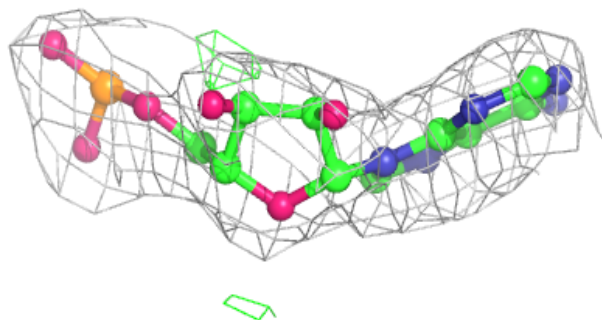
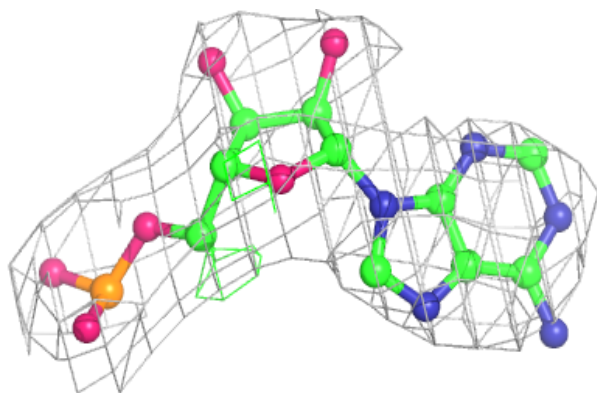
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	AMP	B	2700	22/23	0.91	0.21	81,90,93,93	0
3	AMP	A	700	22/23	0.94	0.16	49,53,56,57	0
2	ZN	B	2701	1/1	0.99	0.10	29,29,29,29	0
2	ZN	A	701	1/1	1.00	0.10	19,19,19,19	0

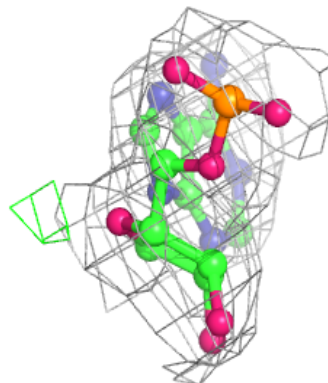
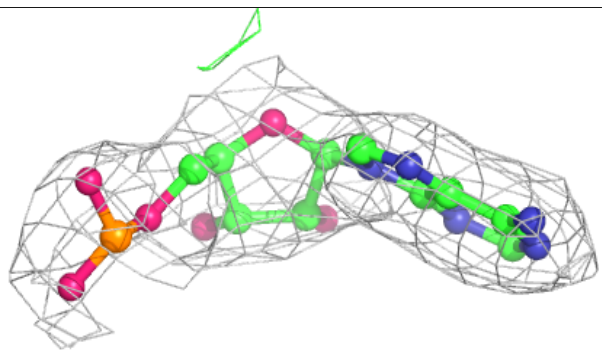
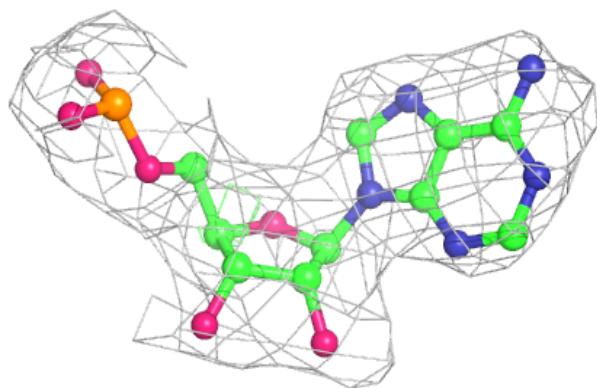
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around AMP B 2700:

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

**Electron density around AMP A 700:**

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



6.5 Other polymers

There are no such residues in this entry.