



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 2, 2026 – 12:37 AM UTC

PDB ID : 1DFC / pdb_00001dfc
Title : CRYSTAL STRUCTURE OF HUMAN FASCIN, AN ACTIN-CROSSLINKING PROTEIN
Authors : Fedorov, A.A.; Fedorov, E.V.; Ono, S.; Matsumura, F.; Almo, S.C.; Burley, S.K.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on : 1999-11-18
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
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
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

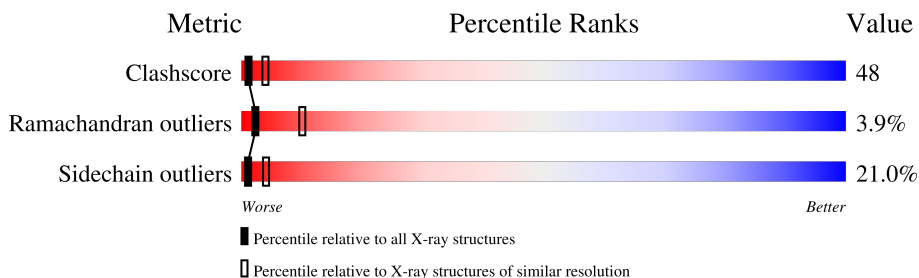
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

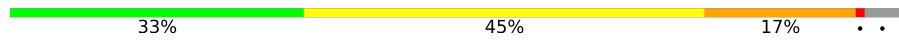

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



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	493	 33% 45% 17% . .
1	B	493	 31% 46% 17% . .

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 7427 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 FASCIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	475	Total 3716	C 2326	N 663	O 714	S 13	0	0	0
1	B	474	Total 3711	C 2323	N 662	O 713	S 13	0	0	0

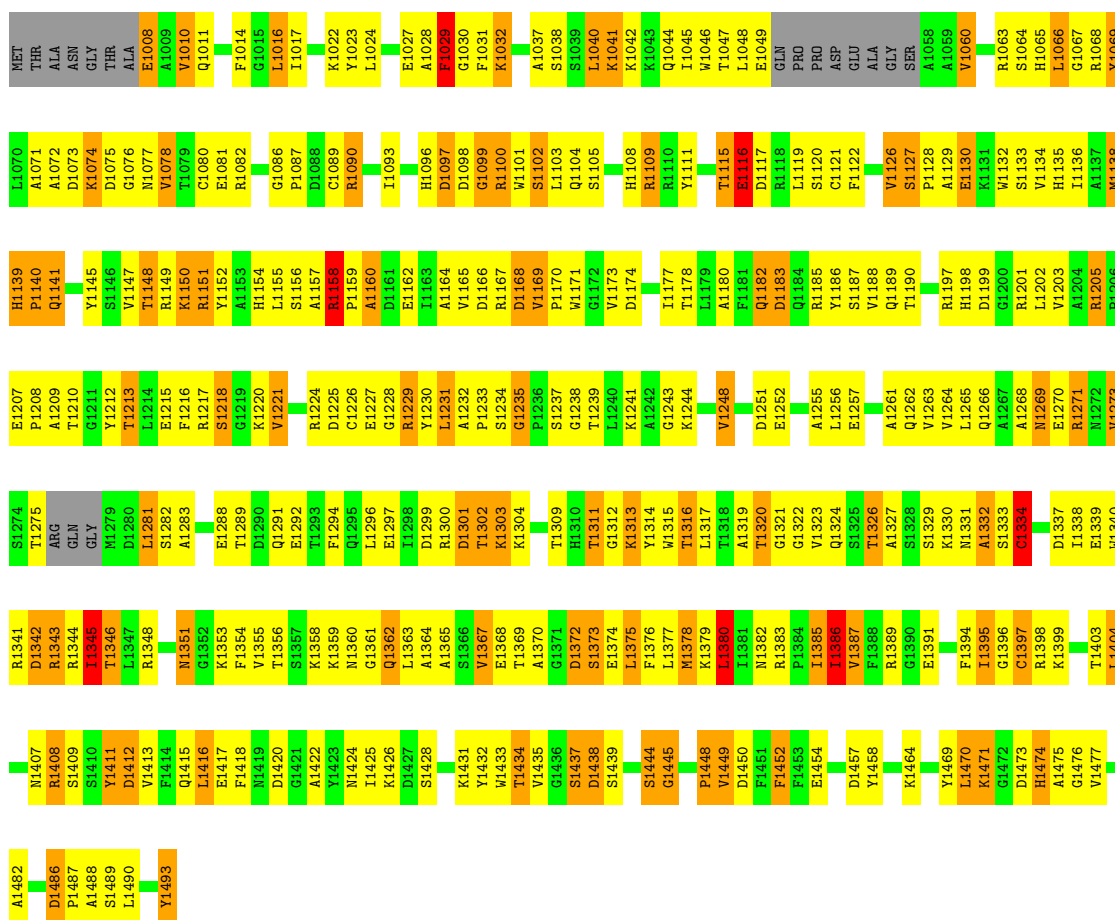
3 Residue-property plots

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: FASCIN

Chain A: 



- Molecule 1: FASCIN

Chain B: 



A2071	V2147	L2214	MET	T2345	Y2411	A2475
A2072	T2148	E2215	D2280	T2346	D2412	G2476
K2073	R2149	F2216	L2281	L2347	V2413	V2477
K2150	R2150	R2217	S2282	R2348	V2414	
R2151	R2151	S2218	A2283	N2351	F2415	A2482
V2077	Y2152	G2219	N2284	N2351	L2416	D2486
V2078	S2156	K2220	Q2285	F2354	E2417	P2487
E2081	A2157	V2221	E2288	V2355	F2418	A2488
R2082	R2158	R2224	T2289	T2356	N2419	S2489
P2085	P2159	D2225	D2290	S2357	D2420	
G2086	A2160	C2226	Q2291	K2358	G2421	A2493
R2090	E2161	G2227	E2292	K2359	A2422	
L2093	E2162	G2228	F2293	N2360		
V2094	L2163	R2229	F2294	G2361	I2425	
A2095	A2164	Y2230	L2296	Q2362	K2426	
H2096	V2165	L2231	L2296	L2363	D2427	
D2097	D2166	A2232	D2299	A2364	S2428	
D2098	R2167	P2233	R2300	A2365	T2429	
G2099	D2168	S2234	D2301	S2366	G2430	
R2100	V2169	G2235	T2302	V2367	K2431	
V2101	W2170	G2236	K2303	E2368	Y2432	
S2102	W2171	S2237	K2303	T2369	W2433	
L2103	G2238	G2238	K2304	A2370	T2434	
Q2104	V2172	T2239	G2371	D2372	V2435	
H2108	D2174	L2240	R2308	S2373	G2436	
R2109	S2175	G2243	T2309	E2374	S2437	
R2110	T2178	K2244	H2310	L2375	D2438	
Y2111	Q2182	V2248	T2311	L2376	S2439	
T2115	D2183	D2251	Q2312	F2377	T2442	
D2116	R2185	E2252	K2313	L2377	S2443	
D2117	R2186	L2253	W2314	W2378	S2444	
S2120	S2187	F2254	W2315	K2379	G2445	
V2126	V2188	A2255	T2316	L2380	G2446	
S2127	Q2189	L2256	L2317	T2381	D2446	
P2128	T2190	E2257	T2318	N2382	T2447	
A2129	A2191	Q2258	A2319	R2383	P2448	
E2130	D2192	S2259	T2320	P2384	V2449	
K2131	H2193	C2260	G2321	I2385	D2450	
S2133	R2197	A2261	G2322	T2386	F2451	
V2134	H2198	Q2262	V2263	V2387	F2452	
H2135	D2199	L2264	V2264	V2387	F2453	
L2136	L2202	L2265	L2265	F2388	E2454	
A2137	W2203	A2267	A2268	R2389	F2455	
H2138	A2204	R2269	R2269	G2390	F2455	
H2139	R2205	E2270	E2270	E2391	C2456	
P2140	P2206	R2271	R2271	F2394	D2457	
Q2141	E2207	N2272	N2272	I2395	D2458	
V2142	P2208	V2273	V2273	G2396	N2458	
Y2145	A2209	S2274	S2274	C2397		
S2146	T2210	T2275	T2275	R2398	A2462	
Y2212	G2211	ARG	ARG	K2399	I2463	
T2213	T2212	GLN	GLN	R2399	V2464	
		GLY	GLY	V2400	V2465	
				T2401		
				D2404		
				D2405		
				A2406		
				N2407		
				R2344		
				R2345		
				R2346		
				R2408		

4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	165.43Å 71.69Å 116.92Å 90.00° 132.17° 90.00°	Depositor
Resolution (Å)	8.00 – 2.90	Depositor
% Data completeness (in resolution range)	83.6 (8.00-2.90)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.184 , 0.268	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	7427	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

5 Model quality i

5.1 Standard geometry i

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	1.18	7/3793 (0.2%)	1.37	33/5126 (0.6%)
1	B	1.18	6/3788 (0.2%)	1.36	39/5119 (0.8%)
All	All	1.18	13/7581 (0.2%)	1.36	72/10245 (0.7%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	1
All	All	0	3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1386	ILE	CA-CB	6.74	1.64	1.54
1	A	1060	VAL	CA-CB	6.36	1.63	1.54
1	B	2386	ILE	CA-CB	6.24	1.64	1.54
1	A	1139	HIS	C-N	-6.11	1.28	1.34
1	A	1183	ASP	CA-C	-5.94	1.46	1.53
1	A	1395	ILE	CA-CB	5.90	1.62	1.54
1	B	2318	THR	CA-CB	-5.78	1.44	1.53
1	A	1345	ILE	CA-CB	5.39	1.62	1.54
1	B	2173	VAL	CA-CB	-5.33	1.48	1.54
1	B	2385	ILE	CA-CB	5.25	1.61	1.54
1	A	1380	LEU	N-CA	5.04	1.52	1.46
1	B	2414	PHE	CA-C	-5.04	1.46	1.53
1	B	2255	ALA	CA-CB	-5.02	1.46	1.53

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1387	VAL	N-CA-C	-9.18	95.70	108.27
1	A	1486	ASP	N-CA-C	-8.48	100.52	108.07
1	B	2263	VAL	N-CA-C	7.98	120.45	108.80
1	B	2028	ALA	N-CA-C	-7.73	103.73	113.01
1	A	1028	ALA	N-CA-C	-7.68	103.80	113.01
1	A	1373	SER	N-CA-C	-7.66	102.12	113.61
1	B	2373	SER	N-CA-C	-7.54	102.30	113.61
1	B	2411	TYR	N-CA-C	7.51	122.26	110.32
1	A	1437	SER	N-CA-C	-7.29	104.37	113.55
1	A	1263	VAL	N-CA-C	7.25	119.38	108.80
1	B	2381	ILE	CB-CA-C	-7.21	104.59	111.44
1	A	1395	ILE	N-CA-C	-7.03	98.34	108.53
1	A	1269	ASN	N-CA-C	-6.83	105.06	113.19
1	A	1301	ASP	N-CA-C	6.81	118.59	111.03
1	B	2381	ILE	N-CA-C	6.77	117.38	111.56
1	B	2066	LEU	N-CA-C	-6.76	102.95	113.02
1	A	1334	CYS	N-CA-C	6.70	121.17	112.92
1	B	2474	HIS	N-CA-C	-6.63	101.74	110.43
1	B	2142	VAL	N-CA-CB	-6.56	104.78	112.32
1	B	2134	VAL	CB-CA-C	-6.46	104.21	111.45
1	B	2387	VAL	N-CA-C	-6.40	98.83	108.17
1	B	2448	PRO	N-CA-C	6.31	120.56	110.21
1	B	2334	CYS	N-CA-C	6.20	120.84	113.16
1	A	1311	THR	N-CA-C	-6.14	102.35	111.81
1	B	2374	GLU	N-CA-C	-6.06	105.93	113.38
1	B	2140	PRO	N-CA-C	6.05	120.97	114.68
1	B	2175	SER	N-CA-C	6.04	119.75	112.38
1	A	1134	VAL	CB-CA-C	-6.02	104.96	111.59
1	A	1409	SER	N-CA-C	-6.02	105.93	113.28
1	A	1372	ASP	N-CA-C	-6.02	103.69	113.19
1	B	2394	PHE	N-CA-C	5.94	117.56	110.19
1	B	2041	LYS	N-CA-C	5.87	116.17	108.07
1	B	2061	CYS	CA-C-N	-5.86	115.23	122.84
1	B	2061	CYS	C-N-CA	-5.86	115.23	122.84
1	B	2253	LEU	N-CA-C	5.83	119.14	109.46
1	A	1412	ASP	CA-C-N	-5.77	115.40	123.13
1	A	1412	ASP	C-N-CA	-5.77	115.40	123.13
1	A	1474	HIS	N-CA-C	-5.75	102.52	110.35
1	B	2069	TYR	N-CA-C	5.75	118.90	109.76
1	A	1046	TRP	CA-C-N	-5.72	114.92	122.99
1	A	1046	TRP	C-N-CA	-5.72	114.92	122.99
1	A	1329	SER	CA-C-N	-5.72	115.41	122.84
1	A	1329	SER	C-N-CA	-5.72	115.41	122.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2401	THR	N-CA-C	5.70	119.04	111.75
1	B	2023	TYR	N-CA-C	5.69	118.23	109.07
1	B	2456	CYS	N-CA-C	5.67	119.93	112.89
1	A	1041	LYS	N-CA-C	5.67	115.89	108.07
1	B	2372	ASP	N-CA-C	-5.64	104.27	113.19
1	A	1263	VAL	CB-CA-C	-5.59	102.54	110.82
1	B	2415	GLN	CA-C-N	-5.55	114.62	122.94
1	B	2415	GLN	C-N-CA	-5.55	114.62	122.94
1	B	2396	GLY	CA-C-N	-5.55	112.59	122.07
1	B	2396	GLY	C-N-CA	-5.55	112.59	122.07
1	A	1411	TYR	N-CA-C	5.54	118.71	110.52
1	A	1448	PRO	N-CA-C	5.48	119.48	110.55
1	B	2486	ASP	N-CA-C	-5.44	101.94	108.25
1	B	2237	SER	N-CA-C	-5.42	106.17	112.89
1	A	1069	TYR	N-CA-C	5.32	118.60	110.20
1	A	1351	ASN	N-CA-C	-5.32	106.98	112.93
1	A	1139	HIS	CA-C-O	5.31	124.17	119.71
1	B	2437	SER	N-CA-C	-5.28	106.52	113.12
1	B	2269	ASN	N-CA-C	-5.28	106.91	113.19
1	B	2251	ASP	N-CA-C	-5.18	106.79	113.01
1	B	2462	ALA	N-CA-C	-5.17	100.97	109.40
1	A	1139	HIS	CA-C-N	-5.14	114.42	120.12
1	A	1139	HIS	C-N-CA	-5.14	114.42	120.12
1	A	1237	SER	N-CA-C	-5.08	107.08	113.28
1	A	1119	LEU	N-CA-C	-5.08	102.00	110.17
1	B	2395	ILE	N-CA-C	-5.07	101.16	108.71
1	B	2025	THR	N-CA-C	5.06	117.99	109.95
1	A	1378	MET	N-CA-C	5.05	116.92	107.99
1	B	2191	ALA	N-CA-C	5.00	118.15	111.75

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1452	PHE	Sidechain
1	A	1493	TYR	Sidechain
1	B	2493	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	3716	0	3599	352	1
1	B	3711	0	3597	357	1
All	All	7427	0	7196	709	1

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 48.

All (709) 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:A:1139:HIS:CE1	1:A:1141:GLN:HG3	1.61	1.36
1:A:1416:LEU:HD12	1:A:1416:LEU:H	1.15	1.12
1:A:1158:ARG:HB2	1:A:1159:PRO:HD3	1.14	1.10
1:B:2158:ARG:HB2	1:B:2159:PRO:HD3	1.11	1.10
1:B:2158:ARG:HB2	1:B:2159:PRO:CD	1.86	1.05
1:A:1269:ASN:OD1	1:A:1271:ARG:HB2	1.58	1.01
1:B:2100:ARG:HB2	1:B:2132:TRP:O	1.59	1.01
1:A:1100:ARG:HB2	1:A:1132:TRP:O	1.61	1.00
1:B:2282:SER:HB3	1:B:2362:GLN:HA	1.43	0.98
1:A:1158:ARG:HB2	1:A:1159:PRO:CD	1.93	0.98
1:B:2043:LYS:HA	1:B:2065:HIS:CD2	1.99	0.97
1:A:1282:SER:HB3	1:A:1362:GLN:HA	1.46	0.96
1:B:2416:LEU:HD12	1:B:2416:LEU:H	1.30	0.96
1:A:1205:ARG:NH1	1:A:1207:GLU:HB3	1.81	0.95
1:A:1127:SER:H	1:A:1130:GLU:HG2	1.29	0.94
1:B:2139:HIS:CE1	1:B:2141:GLN:HG3	2.05	0.91
1:A:1157:ALA:HB3	1:A:1158:ARG:NH1	1.85	0.91
1:A:1139:HIS:HE1	1:A:1141:GLN:CG	1.85	0.89
1:A:1139:HIS:CE1	1:A:1141:GLN:CG	2.53	0.89
1:A:1416:LEU:HD12	1:A:1416:LEU:N	1.81	0.89
1:B:2205:ARG:NH1	1:B:2207:GLU:HB3	1.88	0.88
1:B:2150:LYS:HG3	1:B:2151:ARG:HE	1.36	0.88
1:B:2269:ASN:OD1	1:B:2271:ARG:HB2	1.74	0.88
1:B:2383:ARG:O	1:B:2416:LEU:HD11	1.74	0.87
1:A:1139:HIS:HE1	1:A:1141:GLN:HG3	1.04	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2127:SER:H	1:B:2130:GLU:HG2	1.38	0.87
1:B:2136:ILE:HG23	1:B:2138:MET:SD	2.16	0.86
1:B:2097:ASP:HA	1:B:2224:ARG:NH1	1.92	0.85
1:B:2095:ALA:HB2	1:B:2215:GLU:HG3	1.57	0.84
1:B:2139:HIS:HE1	1:B:2141:GLN:HG3	1.38	0.84
1:A:1299:ASP:OD1	1:A:1302:THR:HG23	1.78	0.83
1:A:1010:VAL:HG12	1:A:1256:LEU:O	1.78	0.82
1:B:2043:LYS:HA	1:B:2065:HIS:HD2	1.43	0.82
1:A:1343:ARG:O	1:A:1344:ARG:HD2	1.79	0.82
1:B:2205:ARG:HH22	1:B:2207:GLU:CD	1.88	0.81
1:A:1398:ARG:HH11	1:A:1403:THR:HG21	1.43	0.81
1:A:1150:LYS:HG3	1:A:1151:ARG:HE	1.43	0.81
1:A:1343:ARG:HG3	1:A:1343:ARG:HH11	1.43	0.80
1:A:1205:ARG:HH22	1:A:1207:GLU:CD	1.89	0.80
1:B:2266:GLN:HG3	1:B:2271:ARG:O	1.80	0.80
1:B:2031:PHE:CD1	1:B:2081:GLU:HG3	2.16	0.80
1:A:1203:VAL:CG2	1:A:1205:ARG:HE	1.95	0.80
1:B:2158:ARG:CB	1:B:2159:PRO:HD3	2.04	0.79
1:A:1205:ARG:HH12	1:A:1207:GLU:HB3	1.46	0.79
1:B:2416:LEU:HD12	1:B:2416:LEU:N	1.97	0.78
1:B:2291:GLN:HB2	1:B:2292:GLU:OE1	1.84	0.78
1:B:2299:ASP:OD1	1:B:2302:THR:HG23	1.84	0.77
1:B:2299:ASP:CG	1:B:2302:THR:HG23	2.09	0.77
1:A:1398:ARG:NH1	1:A:1403:THR:HG21	1.99	0.77
1:A:1354:PHE:HE2	1:A:1370:ALA:HB2	1.49	0.76
1:A:1207:GLU:HB2	1:A:1208:PRO:HD2	1.65	0.76
1:B:2207:GLU:HB2	1:B:2208:PRO:HD2	1.66	0.76
1:A:1203:VAL:HG21	1:A:1205:ARG:HH21	1.50	0.76
1:B:2400:VAL:HG13	1:B:2401:THR:H	1.51	0.75
1:B:2205:ARG:NH2	1:B:2207:GLU:OE1	2.19	0.75
1:A:1031:PHE:CD1	1:A:1081:GLU:HG3	2.22	0.75
1:B:2111:TYR:CE2	1:B:2126:VAL:HG22	2.21	0.74
1:A:1474:HIS:O	1:A:1475:ALA:HB3	1.86	0.74
1:B:2438:ASP:OD1	1:B:2438:ASP:N	2.15	0.74
1:A:1355:VAL:CG1	1:A:1363:LEU:HD13	2.18	0.74
1:B:2324:GLN:HG3	1:B:2326:THR:HB	1.69	0.73
1:A:1063:ARG:HE	1:A:1067:GLY:HA2	1.54	0.73
1:A:1165:VAL:HG12	1:A:1238:GLY:O	1.87	0.73
1:A:1011:GLN:HG3	1:A:1011:GLN:O	1.88	0.72
1:A:1205:ARG:HH22	1:A:1207:GLU:CG	2.01	0.72
1:A:1063:ARG:NE	1:A:1067:GLY:HA2	2.04	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1205:ARG:NH2	1:A:1207:GLU:OE1	2.22	0.72
1:B:2097:ASP:HA	1:B:2224:ARG:HH12	1.53	0.72
1:B:2203:VAL:CG2	1:B:2205:ARG:HE	2.02	0.71
1:A:1339:GLU:O	1:A:1345:ILE:HD12	1.90	0.71
1:A:1299:ASP:CG	1:A:1302:THR:HG23	2.16	0.71
1:A:1299:ASP:OD1	1:A:1302:THR:N	2.23	0.70
1:A:1269:ASN:O	1:A:1270:GLU:HB2	1.91	0.70
1:B:2040:LEU:HD12	1:B:2041:LYS:N	2.06	0.70
1:A:1218:SER:C	1:A:1220:LYS:H	1.99	0.70
1:A:1341:ARG:HH11	1:A:1375:LEU:HD11	1.55	0.70
1:B:2150:LYS:O	1:B:2151:ARG:HD3	1.90	0.70
1:B:2343:ARG:HG3	1:B:2343:ARG:HH11	1.56	0.70
1:A:1027:GLU:HB3	1:A:1029:PHE:HB2	1.72	0.70
1:B:2150:LYS:C	1:B:2151:ARG:HD3	2.16	0.70
1:A:1391:GLU:OE2	1:A:1487:PRO:HB2	1.91	0.70
1:B:2339:GLU:HB3	1:B:2346:THR:CG2	2.22	0.69
1:A:1386:ILE:HD11	1:A:1416:LEU:HG	1.73	0.69
1:B:2010:VAL:HG12	1:B:2256:LEU:O	1.91	0.69
1:B:2342:ASP:O	1:B:2343:ARG:HB2	1.89	0.69
1:A:1040:LEU:HD12	1:A:1041:LYS:N	2.08	0.69
1:A:1354:PHE:CE2	1:A:1370:ALA:HB2	2.27	0.69
1:B:2104:GLN:NE2	1:B:2111:TYR:HE1	1.90	0.69
1:A:1111:TYR:CE2	1:A:1126:VAL:HG22	2.28	0.69
1:A:1203:VAL:HG21	1:A:1205:ARG:HE	1.57	0.69
1:B:2150:LYS:HG3	1:B:2151:ARG:NE	2.08	0.69
1:A:1343:ARG:HD3	1:A:1420:ASP:O	1.93	0.69
1:B:2165:VAL:HG11	1:B:2233:PRO:HB3	1.75	0.69
1:B:2011:GLN:HG3	1:B:2011:GLN:O	1.92	0.68
1:B:2040:LEU:HD12	1:B:2040:LEU:C	2.17	0.68
1:B:2205:ARG:HH12	1:B:2207:GLU:HB3	1.56	0.68
1:A:1342:ASP:O	1:A:1343:ARG:HB2	1.93	0.68
1:A:1343:ARG:HG3	1:A:1343:ARG:NH1	2.08	0.68
1:B:2090:ARG:HH11	1:B:2090:ARG:HB3	1.58	0.68
1:A:1473:ASP:OD1	1:A:1477:VAL:HG22	1.93	0.68
1:A:1362:GLN:HG2	1:A:1363:LEU:N	2.08	0.68
1:A:1313:LYS:HG3	1:A:1327:ALA:O	1.93	0.67
1:B:2454:GLU:OE1	1:B:2464:LYS:HE3	1.95	0.67
1:B:2094:VAL:HB	1:B:2102:SER:HB3	1.77	0.67
1:B:2355:VAL:CG1	1:B:2363:LEU:HD13	2.25	0.67
1:B:2165:VAL:O	1:B:2165:VAL:HG13	1.95	0.67
1:B:2391:GLU:OE2	1:B:2487:PRO:HB2	1.93	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1029:PHE:HB3	1:A:1032:LYS:HG3	1.76	0.67
1:A:1339:GLU:HB3	1:A:1346:THR:HB	1.75	0.67
1:B:2474:HIS:O	1:B:2475:ALA:HB3	1.95	0.67
1:B:2345:ILE:HG22	1:B:2376:PHE:HB2	1.78	0.66
1:B:2203:VAL:HG21	1:B:2205:ARG:HE	1.60	0.66
1:A:1266:GLN:HG3	1:A:1271:ARG:O	1.96	0.66
1:B:2027:GLU:HB3	1:B:2029:PHE:HB2	1.78	0.66
1:B:2269:ASN:OD1	1:B:2269:ASN:C	2.38	0.66
1:B:2299:ASP:OD1	1:B:2302:THR:N	2.29	0.66
1:A:1416:LEU:N	1:A:1416:LEU:CD1	2.58	0.66
1:A:1104:GLN:NE2	1:A:1111:TYR:HE1	1.92	0.65
1:B:2029:PHE:HB3	1:B:2032:LYS:HG3	1.79	0.65
1:A:1316:THR:HG22	1:A:1333:SER:HB3	1.79	0.65
1:B:2398:ARG:HA	1:B:2408:ARG:HH12	1.61	0.65
1:B:2426:LYS:HA	1:B:2431:LYS:O	1.97	0.65
1:B:2457:ASP:OD1	1:B:2458:TYR:N	2.27	0.65
1:A:1183:ASP:C	1:A:1185:ARG:H	2.05	0.65
1:A:1203:VAL:HG21	1:A:1205:ARG:NH2	2.11	0.65
1:A:1136:ILE:HG23	1:A:1138:MET:SD	2.36	0.65
1:A:1339:GLU:HB3	1:A:1346:THR:CG2	2.27	0.65
1:B:2385:ILE:HG23	1:B:2413:VAL:CG1	2.27	0.65
1:A:1031:PHE:CZ	1:A:1068:ARG:CZ	2.80	0.64
1:B:2111:TYR:HE2	1:B:2126:VAL:HG22	1.62	0.64
1:A:1040:LEU:HD12	1:A:1040:LEU:C	2.23	0.64
1:B:2351:ASN:C	1:B:2351:ASN:OD1	2.40	0.64
1:B:2354:PHE:HE2	1:B:2370:ALA:HB2	1.63	0.64
1:B:2127:SER:N	1:B:2130:GLU:HG2	2.12	0.64
1:A:1216:PHE:CD1	1:A:1221:VAL:HG23	2.33	0.64
1:A:1338:ILE:CG2	1:A:1345:ILE:HD11	2.28	0.63
1:A:1182:GLN:NE2	1:A:1210:THR:OG1	2.31	0.63
1:B:2339:GLU:HB3	1:B:2346:THR:HB	1.79	0.63
1:B:2394:PHE:CG	1:B:2411:TYR:HB3	2.34	0.63
1:A:1150:LYS:C	1:A:1151:ARG:HD3	2.23	0.63
1:B:2147:VAL:HG23	1:B:2253:LEU:O	1.99	0.63
1:A:1341:ARG:NH1	1:A:1375:LEU:HD11	2.13	0.63
1:B:2338:ILE:HG21	1:B:2340:TRP:CZ2	2.34	0.63
1:B:2205:ARG:HH22	1:B:2207:GLU:CG	2.12	0.63
1:B:2362:GLN:HG2	1:B:2363:LEU:N	2.13	0.62
1:A:1382:ASN:O	1:A:1383:ARG:HD3	1.98	0.62
1:A:1008:GLU:HG2	1:A:1257:GLU:HB3	1.80	0.62
1:A:1127:SER:N	1:A:1130:GLU:HG2	2.10	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1139:HIS:ND1	1:A:1141:GLN:HG3	2.10	0.62
1:A:1425:ILE:HG21	1:A:1433:TRP:CE2	2.33	0.62
1:B:2316:THR:O	1:B:2323:VAL:HA	2.00	0.62
1:B:2382:ASN:O	1:B:2383:ARG:HD3	2.00	0.62
1:B:2426:LYS:HD3	1:B:2432:TYR:CZ	2.34	0.62
1:B:2203:VAL:HG21	1:B:2205:ARG:HH21	1.62	0.62
1:A:1396:GLY:HA3	1:A:1408:ARG:HD2	1.82	0.62
1:B:2148:THR:HG21	1:B:2251:ASP:CG	2.24	0.62
1:A:1042:LYS:O	1:A:1045:ILE:HG12	2.00	0.62
1:A:1122:PHE:CD1	1:A:1122:PHE:O	2.52	0.61
1:A:1426:LYS:HA	1:A:1431:LYS:O	1.99	0.61
1:B:2218:SER:C	1:B:2220:LYS:H	2.08	0.61
1:B:2294:PHE:CE2	1:B:2309:THR:HG22	2.35	0.61
1:A:1198:HIS:CE1	1:A:1209:ALA:HB1	2.36	0.61
1:B:2343:ARG:O	1:B:2344:ARG:HD2	2.01	0.61
1:B:2252:GLU:N	1:B:2252:GLU:OE2	2.33	0.61
1:B:2294:PHE:HE2	1:B:2309:THR:HG22	1.65	0.61
1:B:2486:ASP:OD1	1:B:2488:ALA:HB3	2.00	0.61
1:A:1183:ASP:C	1:A:1185:ARG:N	2.57	0.61
1:A:1229:ARG:HG2	1:A:1243:GLY:O	2.01	0.61
1:A:1394:PHE:CG	1:A:1411:TYR:HB3	2.36	0.61
1:B:2400:VAL:HG22	1:B:2401:THR:N	2.16	0.61
1:B:2473:ASP:OD1	1:B:2474:HIS:O	2.19	0.61
1:A:1324:GLN:HG3	1:A:1326:THR:HB	1.83	0.60
1:A:1353:LYS:HB2	1:A:1365:ALA:O	2.00	0.60
1:B:2136:ILE:HD12	1:B:2138:MET:SD	2.41	0.60
1:A:1150:LYS:O	1:A:1151:ARG:HD3	2.01	0.60
1:B:2386:ILE:CG1	1:B:2416:LEU:HG	2.29	0.60
1:A:1383:ARG:O	1:A:1416:LEU:HD11	2.01	0.60
1:A:1438:ASP:OD1	1:A:1438:ASP:N	2.21	0.60
1:A:1474:HIS:O	1:A:1475:ALA:CB	2.48	0.60
1:A:1048:LEU:O	1:A:1049:GLU:HG3	2.01	0.60
1:B:2145:TYR:HB3	1:B:2255:ALA:HB3	1.84	0.60
1:B:2311:THR:O	1:B:2311:THR:HG22	2.02	0.60
1:A:1215:GLU:OE2	1:A:1230:TYR:OH	2.20	0.59
1:A:1385:ILE:HG23	1:A:1413:VAL:CG1	2.32	0.59
1:B:2152:TYR:CD2	1:B:2170:PRO:HG3	2.36	0.59
1:A:1416:LEU:HD13	1:A:1416:LEU:O	2.02	0.59
1:A:1165:VAL:HG11	1:A:1233:PRO:HB3	1.83	0.59
1:A:1314:TYR:CZ	1:A:1330:LYS:HE2	2.38	0.59
1:B:2157:ALA:HB3	1:B:2158:ARG:NH1	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2197:ARG:HD2	1:B:2199:ASP:CG	2.27	0.59
1:B:2358:LYS:O	1:B:2359:LYS:C	2.44	0.59
1:B:2048:LEU:HD11	1:B:2060:VAL:HB	1.82	0.59
1:A:1111:TYR:HE2	1:A:1126:VAL:HG22	1.67	0.59
1:A:1217:ARG:CZ	1:A:1248:VAL:HG13	2.32	0.59
1:A:1048:LEU:HD11	1:A:1060:VAL:HB	1.85	0.59
1:A:1225:ASP:OD2	1:A:1229:ARG:NH2	2.36	0.59
1:B:2299:ASP:O	1:B:2303:LYS:HA	2.03	0.59
1:B:2321:GLY:O	1:B:2364:ALA:HB1	2.03	0.59
1:B:2434:THR:HG23	1:B:2449:VAL:CG1	2.32	0.59
1:B:2465:VAL:HG13	1:B:2465:VAL:O	2.01	0.59
1:A:1145:TYR:HB3	1:A:1255:ALA:HB3	1.85	0.59
1:A:1319:ALA:C	1:A:1321:GLY:H	2.10	0.59
1:A:1404:LEU:HD21	1:A:1433:TRP:CE2	2.38	0.58
1:B:2354:PHE:CE2	1:B:2370:ALA:HB2	2.37	0.58
1:A:1354:PHE:HD2	1:A:1370:ALA:HA	1.67	0.58
1:B:2275:THR:HG22	1:B:2281:LEU:HD23	1.85	0.58
1:B:2343:ARG:HD3	1:B:2420:ASP:O	2.03	0.58
1:A:1291:GLN:HB2	1:A:1292:GLU:OE1	2.03	0.58
1:B:2165:VAL:HG12	1:B:2238:GLY:O	2.03	0.58
1:A:1198:HIS:ND1	1:A:1209:ALA:HB1	2.18	0.58
1:A:1314:TYR:OH	1:A:1330:LYS:HE2	2.04	0.58
1:A:1389:ARG:CG	1:A:1394:PHE:CE2	2.86	0.58
1:A:1203:VAL:HG21	1:A:1205:ARG:NE	2.19	0.58
1:B:2386:ILE:HD11	1:B:2416:LEU:HG	1.86	0.58
1:A:1341:ARG:O	1:A:1342:ASP:C	2.46	0.58
1:A:1348:ARG:HB2	1:A:1354:PHE:CE1	2.38	0.58
1:A:1386:ILE:CG1	1:A:1416:LEU:HG	2.33	0.58
1:A:1358:LYS:HB3	1:A:1360:ASN:HD21	1.68	0.57
1:B:2266:GLN:HB3	1:B:2377:LEU:HB3	1.85	0.57
1:B:2269:ASN:O	1:B:2270:GLU:HB2	2.04	0.57
1:A:1379:LYS:HD3	1:A:1418:PHE:CD2	2.39	0.57
1:B:2229:ARG:HG2	1:B:2243:GLY:O	2.04	0.57
1:B:2425:ILE:HG21	1:B:2433:TRP:CE2	2.39	0.57
1:A:1234:SER:OG	1:A:1241:LYS:HD3	2.04	0.57
1:B:2348:ARG:HB2	1:B:2354:PHE:CE1	2.39	0.57
1:A:1203:VAL:CB	1:A:1205:ARG:HE	2.17	0.57
1:B:2238:GLY:O	1:B:2239:THR:C	2.46	0.57
1:A:1040:LEU:HD23	1:A:1135:HIS:CE1	2.39	0.57
1:A:1345:ILE:HG22	1:A:1376:PHE:HB2	1.86	0.57
1:B:2198:HIS:ND1	1:B:2209:ALA:HB1	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2167:ARG:NH1	1:B:2174:ASP:HB2	2.20	0.57
1:A:1205:ARG:HH22	1:A:1207:GLU:HG2	1.67	0.57
1:A:1031:PHE:CE2	1:A:1068:ARG:NE	2.73	0.57
1:A:1316:THR:O	1:A:1323:VAL:HA	2.06	0.56
1:A:1474:HIS:C	1:A:1476:GLY:H	2.13	0.56
1:B:2148:THR:HG21	1:B:2251:ASP:OD2	2.05	0.56
1:B:2217:ARG:CZ	1:B:2248:VAL:HG13	2.34	0.56
1:B:2324:GLN:CG	1:B:2326:THR:HB	2.35	0.56
1:A:1331:ASN:O	1:A:1332:ALA:C	2.47	0.56
1:A:1486:ASP:HB2	1:A:1487:PRO:HD2	1.88	0.56
1:B:2316:THR:N	1:B:2324:GLN:O	2.39	0.56
1:B:2398:ARG:NH1	1:B:2405:ASP:OD1	2.37	0.56
1:A:1049:GLU:OE2	1:A:1063:ARG:HG3	2.05	0.56
1:A:1205:ARG:NH2	1:A:1207:GLU:HG2	2.21	0.56
1:A:1269:ASN:HD21	1:A:1283:ALA:CB	2.19	0.56
1:A:1386:ILE:CD1	1:A:1416:LEU:HG	2.35	0.56
1:A:1090:ARG:HH11	1:A:1090:ARG:HB3	1.70	0.56
1:B:2358:LYS:HB3	1:B:2360:ASN:HD21	1.69	0.56
1:B:2422:ALA:HB1	1:B:2450:ASP:HB3	1.88	0.56
1:B:2097:ASP:HA	1:B:2224:ARG:CZ	2.35	0.56
1:A:1207:GLU:CB	1:A:1208:PRO:HD2	2.36	0.56
1:A:1313:LYS:CG	1:A:1327:ALA:O	2.53	0.56
1:A:1294:PHE:CE2	1:A:1309:THR:HG22	2.41	0.56
1:A:1358:LYS:O	1:A:1359:LYS:C	2.48	0.56
1:B:2203:VAL:HG21	1:B:2205:ARG:NH2	2.20	0.56
1:A:1159:PRO:O	1:A:1160:ALA:O	2.23	0.56
1:A:1165:VAL:HG13	1:A:1165:VAL:O	2.06	0.56
1:B:2203:VAL:HG21	1:B:2205:ARG:NE	2.21	0.55
1:A:1096:HIS:NE2	1:A:1102:SER:HB2	2.22	0.55
1:B:2271:ARG:HG2	1:B:2271:ARG:HH11	1.71	0.55
1:B:2316:THR:HG22	1:B:2333:SER:HB3	1.89	0.55
1:B:2474:HIS:C	1:B:2476:GLY:H	2.14	0.55
1:A:1294:PHE:HE2	1:A:1309:THR:HG22	1.72	0.55
1:B:2183:ASP:C	1:B:2185:ARG:N	2.63	0.55
1:A:1398:ARG:HD2	1:A:1403:THR:HB	1.88	0.55
1:B:2048:LEU:O	1:B:2049:GLU:HG3	2.07	0.55
1:B:2188:VAL:HG12	1:B:2188:VAL:O	2.05	0.55
1:B:2041:LYS:O	1:B:2045:ILE:HG23	2.06	0.55
1:A:1271:ARG:HG2	1:A:1271:ARG:HH11	1.71	0.55
1:B:2063:ARG:NE	1:B:2067:GLY:HA2	2.22	0.55
1:B:2159:PRO:O	1:B:2160:ALA:O	2.25	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2398:ARG:HA	1:B:2408:ARG:NH1	2.22	0.55
1:A:1238:GLY:O	1:A:1239:THR:C	2.49	0.55
1:B:2398:ARG:O	1:B:2400:VAL:N	2.39	0.55
1:A:1041:LYS:O	1:A:1045:ILE:HG23	2.07	0.55
1:A:1158:ARG:CB	1:A:1159:PRO:HD3	2.10	0.55
1:B:2093:ILE:HD13	1:B:2101:TRP:CH2	2.42	0.55
1:B:2198:HIS:CE1	1:B:2209:ALA:HB1	2.42	0.55
1:B:2207:GLU:CB	1:B:2208:PRO:HD2	2.35	0.54
1:A:1150:LYS:HG3	1:A:1151:ARG:NE	2.17	0.54
1:A:1197:ARG:HD2	1:A:1199:ASP:CG	2.32	0.54
1:A:1315:TRP:O	1:A:1334:CYS:HB3	2.06	0.54
1:B:2339:GLU:HB3	1:B:2346:THR:HG22	1.89	0.54
1:A:1180:ALA:HA	1:A:1411:TYR:OH	2.07	0.54
1:B:2416:LEU:N	1:B:2416:LEU:CD1	2.70	0.54
1:B:2469:TYR:HB2	1:B:2482:ALA:HB3	1.89	0.54
1:A:1205:ARG:CZ	1:A:1207:GLU:HB3	2.38	0.54
1:B:2259:SER:HB3	1:B:2383:ARG:HH12	1.72	0.54
1:B:2096:HIS:O	1:B:2097:ASP:C	2.50	0.54
1:A:1203:VAL:HB	1:A:1205:ARG:HE	1.73	0.54
1:A:1322:GLY:HA2	1:A:1364:ALA:HB2	1.89	0.54
1:A:1331:ASN:O	1:A:1333:SER:N	2.42	0.54
1:A:1422:ALA:HB1	1:A:1450:ASP:HB3	1.90	0.54
1:A:1338:ILE:HG23	1:A:1345:ILE:HD11	1.89	0.53
1:A:1339:GLU:HB3	1:A:1346:THR:CB	2.38	0.53
1:B:2063:ARG:HG2	1:B:2069:TYR:CE1	2.43	0.53
1:B:2339:GLU:HB3	1:B:2346:THR:CB	2.37	0.53
1:A:1319:ALA:C	1:A:1321:GLY:N	2.64	0.53
1:A:1030:GLY:O	1:A:1031:PHE:C	2.51	0.53
1:A:1398:ARG:HG3	1:A:1408:ARG:HH12	1.73	0.53
1:B:2030:GLY:O	1:B:2032:LYS:HG2	2.07	0.53
1:A:1269:ASN:ND2	1:A:1283:ALA:HB3	2.23	0.53
1:B:2314:TYR:OH	1:B:2330:LYS:HE2	2.09	0.53
1:B:2049:GLU:OE2	1:B:2063:ARG:HG3	2.09	0.53
1:A:1304:LYS:HG2	1:A:1337:ASP:OD2	2.09	0.53
1:A:1477:VAL:HG23	1:A:1477:VAL:O	2.08	0.53
1:B:2338:ILE:CG2	1:B:2345:ILE:HD11	2.39	0.53
1:B:2434:THR:CG2	1:B:2449:VAL:HG11	2.38	0.53
1:B:2213:THR:OG1	1:B:2224:ARG:HB3	2.09	0.53
1:B:2355:VAL:HG13	1:B:2363:LEU:HD13	1.91	0.53
1:B:2474:HIS:O	1:B:2475:ALA:CB	2.57	0.53
1:A:1072:ALA:HA	1:A:1077:ASN:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1185:ARG:NH2	1:A:1226:CYS:HA	2.23	0.53
1:B:2065:HIS:HE1	1:B:2066:LEU:HD21	1.74	0.53
1:A:1269:ASN:CG	1:A:1271:ARG:HB2	2.32	0.52
1:A:1136:ILE:HD12	1:A:1138:MET:SD	2.50	0.52
1:A:1229:ARG:CZ	1:A:1229:ARG:HB2	2.39	0.52
1:A:1275:THR:HG22	1:A:1281:LEU:HD23	1.92	0.52
1:A:1281:LEU:HD13	1:A:1315:TRP:CE2	2.45	0.52
1:B:2282:SER:HB3	1:B:2362:GLN:CA	2.29	0.52
1:B:2152:TYR:CG	1:B:2170:PRO:HG3	2.44	0.52
1:A:1377:LEU:HD23	1:A:1377:LEU:O	2.09	0.52
1:A:1348:ARG:NE	1:A:1354:PHE:HE1	2.08	0.52
1:B:2063:ARG:HD3	1:B:2069:TYR:CE2	2.45	0.52
1:B:2081:GLU:O	1:B:2081:GLU:HG2	2.10	0.52
1:B:2216:PHE:CD1	1:B:2221:VAL:HG23	2.45	0.52
1:A:1351:ASN:C	1:A:1351:ASN:OD1	2.52	0.52
1:B:2252:GLU:N	1:B:2252:GLU:CD	2.68	0.52
1:A:1385:ILE:HG23	1:A:1413:VAL:HG13	1.90	0.52
1:B:2072:ALA:HA	1:B:2077:ASN:O	2.10	0.52
1:B:2149:ARG:HD2	1:B:2233:PRO:HB2	1.92	0.52
1:A:1115:THR:O	1:A:1116:GLU:C	2.53	0.51
1:A:1167:ARG:NH2	1:A:1171:TRP:HB3	2.25	0.51
1:A:1205:ARG:NH2	1:A:1207:GLU:CG	2.71	0.51
1:A:1358:LYS:HB3	1:A:1360:ASN:ND2	2.25	0.51
1:B:2010:VAL:CG1	1:B:2256:LEU:O	2.59	0.51
1:B:2346:THR:HG22	1:B:2346:THR:O	2.09	0.51
1:A:1457:ASP:OD1	1:A:1458:TYR:N	2.35	0.51
1:A:1127:SER:H	1:A:1130:GLU:CG	2.11	0.51
1:A:1127:SER:O	1:A:1128:PRO:C	2.53	0.51
1:B:2342:ASP:O	1:B:2343:ARG:CB	2.57	0.51
1:A:1201:ARG:HG2	1:A:1202:LEU:H	1.74	0.51
1:A:1266:GLN:HB3	1:A:1377:LEU:HB3	1.92	0.51
1:A:1299:ASP:O	1:A:1303:LYS:HA	2.10	0.51
1:A:1289:THR:C	1:A:1291:GLN:N	2.68	0.51
1:B:2205:ARG:NH2	1:B:2207:GLU:HG2	2.26	0.51
1:A:1010:VAL:HG12	1:A:1256:LEU:C	2.35	0.51
1:A:1389:ARG:HG2	1:A:1394:PHE:CE2	2.45	0.51
1:B:2473:ASP:OD1	1:B:2477:VAL:HG22	2.10	0.51
1:B:2136:ILE:CG2	1:B:2138:MET:SD	2.95	0.51
1:B:2031:PHE:CZ	1:B:2068:ARG:CZ	2.93	0.51
1:B:2203:VAL:CB	1:B:2205:ARG:HE	2.23	0.51
1:A:1339:GLU:CB	1:A:1346:THR:HG22	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2281:LEU:HD13	1:B:2315:TRP:CE2	2.46	0.50
1:B:2379:LYS:HB2	1:B:2418:PHE:CZ	2.47	0.50
1:A:1185:ARG:HH22	1:A:1226:CYS:HA	1.75	0.50
1:A:1317:LEU:HD12	1:A:1322:GLY:O	2.10	0.50
1:A:1469:TYR:HB2	1:A:1482:ALA:HB3	1.93	0.50
1:B:2065:HIS:CE1	1:B:2066:LEU:HD21	2.47	0.50
1:B:2269:ASN:CG	1:B:2271:ARG:HB2	2.36	0.50
1:B:2182:GLN:NE2	1:B:2210:THR:OG1	2.44	0.50
1:B:2269:ASN:OD1	1:B:2271:ARG:N	2.45	0.50
1:B:2343:ARG:HH11	1:B:2343:ARG:CG	2.22	0.50
1:A:1154:HIS:CE1	1:A:1164:ALA:HB3	2.47	0.50
1:A:1342:ASP:HB2	1:A:1452:PHE:CG	2.46	0.50
1:B:2339:GLU:O	1:B:2345:ILE:HD12	2.10	0.50
1:B:2358:LYS:HB3	1:B:2360:ASN:ND2	2.27	0.50
1:A:1069:TYR:N	1:A:1069:TYR:CD2	2.78	0.50
1:A:1082:ARG:HH21	1:A:1086:GLY:HA3	1.77	0.50
1:A:1183:ASP:O	1:A:1185:ARG:N	2.45	0.50
1:A:1269:ASN:OD1	1:A:1271:ARG:CB	2.45	0.50
1:B:2205:ARG:O	1:B:2205:ARG:HG2	2.11	0.50
1:A:1397:CYS:HB2	1:A:1412:ASP:OD1	2.12	0.50
1:B:2183:ASP:C	1:B:2185:ARG:H	2.18	0.50
1:A:1045:ILE:HD11	1:A:1065:HIS:CD2	2.46	0.50
1:A:1471:LYS:HB2	1:A:1489:SER:HB3	1.93	0.50
1:B:2274:SER:HB3	1:B:2292:GLU:HG3	1.94	0.50
1:B:2432:TYR:CD1	1:B:2448:PRO:HB3	2.47	0.50
1:A:1387:VAL:CG2	1:A:1413:VAL:HG22	2.42	0.49
1:B:2314:TYR:CZ	1:B:2330:LYS:HE2	2.47	0.49
1:A:1010:VAL:CG1	1:A:1256:LEU:HB2	2.42	0.49
1:A:1339:GLU:CB	1:A:1346:THR:CG2	2.90	0.49
1:B:2093:ILE:HG21	1:B:2101:TRP:CE2	2.48	0.49
1:B:2198:HIS:HD1	1:B:2209:ALA:HB1	1.77	0.49
1:B:2263:VAL:HG21	1:B:2378:MET:HE2	1.94	0.49
1:A:1149:ARG:HD2	1:A:1233:PRO:HB2	1.93	0.49
1:B:2205:ARG:HH22	1:B:2207:GLU:HG2	1.76	0.49
1:B:2205:ARG:NH1	1:B:2207:GLU:OE1	2.45	0.49
1:B:2308:ARG:HB2	1:B:2314:TYR:CE2	2.48	0.49
1:A:1148:THR:HG21	1:A:1251:ASP:CG	2.36	0.49
1:A:1148:THR:HG21	1:A:1251:ASP:OD2	2.12	0.49
1:A:1149:ARG:HD2	1:A:1233:PRO:CB	2.43	0.49
1:A:1224:ARG:HG3	1:A:1230:TYR:CE2	2.48	0.49
1:B:2416:LEU:HD13	1:B:2416:LEU:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2486:ASP:HB2	1:B:2487:PRO:HD2	1.94	0.49
1:A:1486:ASP:OD1	1:A:1488:ALA:HB3	2.12	0.49
1:B:2150:LYS:O	1:B:2150:LYS:CG	2.61	0.49
1:B:2151:ARG:HD3	1:B:2151:ARG:N	2.19	0.49
1:B:2170:PRO:HA	1:B:2175:SER:OG	2.13	0.49
1:A:1205:ARG:HH12	1:A:1207:GLU:CB	2.19	0.49
1:A:1387:VAL:HG22	1:A:1413:VAL:HG22	1.95	0.49
1:A:1437:SER:C	1:A:1439:SER:H	2.20	0.49
1:B:2260:CYS:O	1:B:2261:ALA:C	2.54	0.49
1:A:1252:GLU:N	1:A:1252:GLU:OE2	2.47	0.48
1:A:1417:GLU:OE1	1:A:1432:TYR:OH	2.28	0.48
1:B:2008:GLU:O	1:B:2258:GLN:HG2	2.13	0.48
1:B:2100:ARG:CB	1:B:2132:TRP:O	2.48	0.48
1:B:2186:TYR:O	1:B:2212:TYR:N	2.44	0.48
1:B:2274:SER:CB	1:B:2292:GLU:HG3	2.43	0.48
1:B:2275:THR:HG22	1:B:2281:LEU:CD2	2.43	0.48
1:B:2331:ASN:O	1:B:2332:ALA:C	2.54	0.48
1:A:1159:PRO:O	1:A:1160:ALA:C	2.56	0.48
1:A:1343:ARG:C	1:A:1344:ARG:HD2	2.38	0.48
1:B:2427:ASP:C	1:B:2427:ASP:OD1	2.55	0.48
1:A:1269:ASN:OD1	1:A:1269:ASN:C	2.56	0.48
1:A:1339:GLU:HB3	1:A:1346:THR:HG22	1.95	0.48
1:B:2361:GLY:C	1:B:2362:GLN:O	2.54	0.48
1:A:1149:ARG:NH2	1:A:1235:GLY:O	2.47	0.48
1:A:1321:GLY:O	1:A:1364:ALA:HB1	2.14	0.48
1:B:2342:ASP:HB2	1:B:2452:PHE:CD2	2.49	0.48
1:A:1369:THR:O	1:A:1370:ALA:C	2.57	0.48
1:B:2042:LYS:O	1:B:2045:ILE:HG12	2.13	0.48
1:B:2090:ARG:HH11	1:B:2090:ARG:CB	2.24	0.48
1:B:2384:PRO:O	1:B:2385:ILE:HD13	2.14	0.48
1:A:1022:LYS:HA	1:A:1037:ALA:O	2.13	0.48
1:A:1269:ASN:HD21	1:A:1283:ALA:HB3	1.77	0.48
1:B:2063:ARG:HG2	1:B:2069:TYR:CZ	2.49	0.48
1:B:2203:VAL:HB	1:B:2205:ARG:HE	1.78	0.48
1:B:2434:THR:HG23	1:B:2449:VAL:HG11	1.95	0.48
1:A:1261:ALA:HB2	1:A:1493:TYR:CE2	2.49	0.48
1:B:2115:THR:HG23	1:B:2116:GLU:N	2.28	0.48
1:B:2407:ASN:ND2	1:B:2476:GLY:HA3	2.29	0.48
1:A:1156:SER:HB2	1:A:1164:ALA:HB2	1.95	0.48
1:B:2212:TYR:CZ	1:B:2231:LEU:HD21	2.49	0.48
1:B:2389:ARG:CG	1:B:2394:PHE:CE2	2.97	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1198:HIS:HD1	1:A:1209:ALA:HB1	1.79	0.47
1:A:1215:GLU:OE2	1:A:1230:TYR:CZ	2.67	0.47
1:A:1343:ARG:NH1	1:A:1343:ARG:CG	2.75	0.47
1:B:2095:ALA:HB2	1:B:2215:GLU:CG	2.36	0.47
1:A:1355:VAL:HG13	1:A:1363:LEU:HD13	1.93	0.47
1:A:1373:SER:OG	1:A:1374:GLU:OE2	2.27	0.47
1:B:2197:ARG:HB3	1:B:2199:ASP:OD1	2.15	0.47
1:B:2366:SER:O	1:B:2367:VAL:C	2.58	0.47
1:A:1158:ARG:HH11	1:A:1158:ARG:H	1.62	0.47
1:B:2017:ILE:HA	1:B:2022:LYS:O	2.14	0.47
1:B:2313:LYS:HG3	1:B:2327:ALA:O	2.14	0.47
1:B:2319:ALA:C	1:B:2321:GLY:H	2.22	0.47
1:A:1078:VAL:HG12	1:A:1120:SER:HA	1.96	0.47
1:B:2343:ARG:C	1:B:2344:ARG:HD2	2.39	0.47
1:A:1048:LEU:HA	1:A:1048:LEU:HD12	1.48	0.47
1:B:2259:SER:CB	1:B:2383:ARG:HH12	2.28	0.47
1:A:1197:ARG:HA	1:A:1210:THR:HG22	1.95	0.47
1:A:1289:THR:C	1:A:1291:GLN:H	2.21	0.47
1:B:2156:SER:HB2	1:B:2164:ALA:HB2	1.95	0.47
1:B:2225:ASP:OD1	1:B:2225:ASP:C	2.57	0.47
1:B:2382:ASN:O	1:B:2382:ASN:CG	2.57	0.47
1:B:2385:ILE:CD1	1:B:2415:GLN:HB3	2.44	0.47
1:A:1339:GLU:OE2	1:A:1346:THR:HG21	2.15	0.47
1:B:2135:HIS:C	1:B:2135:HIS:CD2	2.93	0.47
1:B:2197:ARG:HA	1:B:2210:THR:HG22	1.96	0.47
1:B:2205:ARG:NH2	1:B:2207:GLU:CG	2.78	0.47
1:A:1064:SER:C	1:A:1066:LEU:H	2.23	0.47
1:A:1132:TRP:CD1	1:A:1132:TRP:N	2.82	0.47
1:A:1269:ASN:O	1:A:1270:GLU:CB	2.57	0.47
1:B:2100:ARG:N	1:B:2100:ARG:CD	2.77	0.47
1:B:2386:ILE:CD1	1:B:2416:LEU:HG	2.44	0.47
1:A:1426:LYS:HG3	1:A:1431:LYS:O	2.15	0.47
1:B:2264:VAL:HG11	1:B:2288:GLU:HG2	1.97	0.47
1:B:2063:ARG:HE	1:B:2067:GLY:HA2	1.79	0.46
1:B:2109:ARG:HH11	1:B:2109:ARG:CG	2.28	0.46
1:B:2289:THR:C	1:B:2291:GLN:N	2.73	0.46
1:A:1127:SER:O	1:A:1129:ALA:N	2.47	0.46
1:A:1316:THR:N	1:A:1324:GLN:O	2.48	0.46
1:A:1074:LYS:HZ2	1:A:1108:HIS:HA	1.79	0.46
1:A:1096:HIS:O	1:A:1097:ASP:C	2.58	0.46
1:A:1150:LYS:O	1:A:1150:LYS:CG	2.62	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2093:ILE:HG23	1:B:2101:TRP:CD2	2.51	0.46
1:B:2300:ARG:NH2	1:B:2458:TYR:CZ	2.84	0.46
1:B:2367:VAL:CG1	1:B:2369:THR:O	2.62	0.46
1:A:1063:ARG:HG2	1:A:1069:TYR:CE1	2.50	0.46
1:A:1167:ARG:NH1	1:A:1174:ASP:HB2	2.31	0.46
1:A:1207:GLU:HB2	1:A:1208:PRO:CD	2.42	0.46
1:B:2069:TYR:N	1:B:2069:TYR:CD2	2.83	0.46
1:B:2446:ASP:OD1	1:B:2446:ASP:N	2.45	0.46
1:A:1017:ILE:HA	1:A:1022:LYS:O	2.16	0.46
1:A:1076:GLY:HA2	1:A:1121:CYS:O	2.16	0.46
1:A:1008:GLU:CG	1:A:1257:GLU:HB3	2.45	0.46
1:A:1030:GLY:O	1:A:1032:LYS:HG2	2.16	0.46
1:A:1299:ASP:O	1:A:1300:ARG:C	2.59	0.46
1:A:1317:LEU:HD12	1:A:1317:LEU:HA	1.59	0.46
1:B:2205:ARG:HH12	1:B:2207:GLU:CB	2.25	0.46
1:A:1016:LEU:O	1:A:1023:TYR:HA	2.15	0.46
1:A:1201:ARG:HG2	1:A:1202:LEU:N	2.31	0.46
1:B:2045:ILE:O	1:B:2045:ILE:HG13	2.16	0.46
1:B:2471:LYS:HB2	1:B:2489:SER:HB3	1.98	0.46
1:A:1473:ASP:OD1	1:A:1474:HIS:O	2.34	0.46
1:B:2142:VAL:HG21	1:B:2256:LEU:HD22	1.98	0.46
1:B:2465:VAL:O	1:B:2465:VAL:CG1	2.63	0.46
1:A:1264:VAL:HG21	1:A:1288:GLU:HG2	1.96	0.46
1:B:2048:LEU:HD11	1:B:2060:VAL:CB	2.46	0.46
1:A:1269:ASN:OD1	1:A:1271:ARG:N	2.49	0.46
1:A:1041:LYS:H	1:A:1044:GLN:HB2	1.81	0.45
1:A:1105:SER:O	1:A:1109:ARG:N	2.45	0.45
1:A:1340:TRP:HA	1:A:1345:ILE:CD1	2.46	0.45
1:A:1367:VAL:CG1	1:A:1368:GLU:N	2.76	0.45
1:B:2024:LEU:C	1:B:2024:LEU:CD2	2.89	0.45
1:B:2379:LYS:HB2	1:B:2418:PHE:CE2	2.51	0.45
1:B:2389:ARG:HG3	1:B:2394:PHE:CE2	2.50	0.45
1:A:1322:GLY:HA2	1:A:1364:ALA:CB	2.46	0.45
1:A:1426:LYS:HD3	1:A:1432:TYR:CZ	2.52	0.45
1:B:2063:ARG:CG	1:B:2069:TYR:CZ	3.00	0.45
1:B:2071:ALA:O	1:B:2078:VAL:HA	2.17	0.45
1:A:1187:SER:HB3	1:A:1210:THR:O	2.16	0.45
1:A:1282:SER:CB	1:A:1362:GLN:HA	2.33	0.45
1:B:2284:ASN:ND2	1:B:2285:GLN:HG2	2.31	0.45
1:B:2319:ALA:C	1:B:2321:GLY:N	2.74	0.45
1:A:1073:ASP:C	1:A:1073:ASP:OD1	2.58	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1093:ILE:HD13	1:A:1101:TRP:CH2	2.52	0.45
1:A:1111:TYR:N	1:A:1111:TYR:CD1	2.83	0.45
1:B:2031:PHE:CE2	1:B:2068:ARG:NE	2.83	0.45
1:B:2284:ASN:C	1:B:2284:ASN:HD22	2.24	0.45
1:B:2173:VAL:O	1:B:2174:ASP:C	2.60	0.45
1:B:2218:SER:C	1:B:2220:LYS:N	2.74	0.45
1:B:2343:ARG:NH2	1:B:2450:ASP:OD2	2.50	0.45
1:B:2381:ILE:HG13	1:B:2382:ASN:N	2.32	0.45
1:A:1150:LYS:NZ	1:A:1168:ASP:OD1	2.48	0.45
1:A:1398:ARG:CG	1:A:1408:ARG:HH12	2.28	0.45
1:B:2141:GLN:C	1:B:2142:VAL:CG1	2.89	0.45
1:B:2339:GLU:CB	1:B:2346:THR:HG22	2.47	0.45
1:B:2379:LYS:HD3	1:B:2418:PHE:CD2	2.52	0.45
1:A:1262:GLN:HB2	1:A:1382:ASN:CG	2.42	0.45
1:A:1311:THR:O	1:A:1312:GLY:C	2.58	0.45
1:B:2224:ARG:HG3	1:B:2230:TYR:CE2	2.52	0.45
1:A:1361:GLY:C	1:A:1362:GLN:O	2.55	0.45
1:B:2275:THR:CG2	1:B:2281:LEU:CD2	2.94	0.45
1:A:1297:GLU:OE1	1:A:1330:LYS:NZ	2.32	0.45
1:A:1444:SER:HB2	1:A:1445:GLY:H	1.47	0.45
1:B:2149:ARG:HD2	1:B:2233:PRO:CB	2.46	0.45
1:A:1282:SER:HB2	1:A:1361:GLY:C	2.42	0.44
1:B:2082:ARG:HH21	1:B:2086:GLY:HA3	1.83	0.44
1:B:2205:ARG:CZ	1:B:2207:GLU:OE1	2.65	0.44
1:B:2422:ALA:CB	1:B:2450:ASP:HB3	2.47	0.44
1:A:1041:LYS:NZ	1:A:1407:ASN:HB2	2.32	0.44
1:B:2069:TYR:CE1	1:B:2085:PRO:HG3	2.52	0.44
1:B:2141:GLN:C	1:B:2142:VAL:HG13	2.42	0.44
1:B:2271:ARG:HH11	1:B:2271:ARG:CG	2.30	0.44
1:B:2227:GLU:HB2	1:B:2229:ARG:HE	1.83	0.44
1:A:1126:VAL:HA	1:A:1130:GLU:HG3	1.99	0.44
1:A:1354:PHE:CD2	1:A:1370:ALA:HA	2.50	0.44
1:B:2065:HIS:CE1	1:B:2066:LEU:CD2	3.01	0.44
1:B:2095:ALA:HB1	1:B:2224:ARG:HD2	2.00	0.44
1:B:2338:ILE:HG23	1:B:2345:ILE:HD11	1.98	0.44
1:A:1203:VAL:HG21	1:A:1205:ARG:CZ	2.46	0.44
1:B:2017:ILE:CG2	1:B:2021:ASN:HA	2.48	0.44
1:B:2169:VAL:HA	1:B:2170:PRO:HD3	1.82	0.44
1:A:1197:ARG:HE	1:A:1207:GLU:CD	2.25	0.44
1:A:1213:THR:OG1	1:A:1224:ARG:HB3	2.17	0.44
1:A:1111:TYR:N	1:A:1111:TYR:HD1	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1139:HIS:ND1	1:A:1140:PRO:HD2	2.33	0.44
1:A:1265:LEU:HB2	1:A:1273:VAL:HG13	1.99	0.44
1:B:2338:ILE:HG21	1:B:2340:TRP:CE2	2.52	0.44
1:B:2459:ASN:CG	1:B:2459:ASN:O	2.60	0.44
1:A:1027:GLU:C	1:A:1029:PHE:N	2.76	0.44
1:A:1385:ILE:HD13	1:A:1385:ILE:HA	1.66	0.44
1:B:2115:THR:O	1:B:2116:GLU:C	2.61	0.44
1:B:2331:ASN:O	1:B:2333:SER:N	2.51	0.44
1:A:1319:ALA:O	1:A:1321:GLY:N	2.51	0.44
1:A:1470:LEU:HA	1:A:1470:LEU:HD12	1.75	0.44
1:B:2043:LYS:HD2	1:B:2065:HIS:NE2	2.33	0.44
1:B:2074:LYS:HG2	1:B:2108:HIS:ND1	2.33	0.44
1:B:2426:LYS:HG3	1:B:2431:LYS:O	2.17	0.44
1:B:2159:PRO:O	1:B:2160:ALA:C	2.61	0.43
1:A:1017:ILE:HG23	1:A:1022:LYS:O	2.17	0.43
1:A:1063:ARG:HG2	1:A:1069:TYR:CZ	2.52	0.43
1:A:1155:LEU:HD23	1:A:1156:SER:N	2.33	0.43
1:A:1271:ARG:HH11	1:A:1271:ARG:CG	2.29	0.43
1:B:2096:HIS:NE2	1:B:2102:SER:HB2	2.33	0.43
1:B:2100:ARG:HB2	1:B:2101:TRP:H	1.45	0.43
1:A:1252:GLU:N	1:A:1252:GLU:CD	2.76	0.43
1:B:2048:LEU:HD12	1:B:2048:LEU:HA	1.77	0.43
1:B:2339:GLU:CB	1:B:2346:THR:CG2	2.94	0.43
1:B:2395:ILE:HA	1:B:2405:ASP:O	2.17	0.43
1:B:2268:ALA:C	1:B:2270:GLU:H	2.26	0.43
1:B:2280:ASP:O	1:B:2281:LEU:C	2.61	0.43
1:B:2289:THR:C	1:B:2291:GLN:H	2.26	0.43
1:A:1186:TYR:O	1:A:1212:TYR:N	2.51	0.43
1:B:2094:VAL:HB	1:B:2102:SER:CB	2.47	0.43
1:B:2284:ASN:ND2	1:B:2284:ASN:C	2.76	0.43
1:B:2296:LEU:CD1	1:B:2378:MET:HE1	2.49	0.43
1:B:2343:ARG:HG2	1:B:2452:PHE:HE2	1.82	0.43
1:B:2367:VAL:CG1	1:B:2368:GLU:N	2.81	0.43
1:A:1045:ILE:HG13	1:A:1045:ILE:O	2.18	0.43
1:A:1232:ALA:HB1	1:A:1233:PRO:HD2	2.00	0.43
1:A:1324:GLN:CG	1:A:1326:THR:HB	2.49	0.43
1:A:1087:PRO:C	1:A:1089:CYS:H	2.26	0.43
1:B:2151:ARG:HD3	1:B:2151:ARG:HA	1.57	0.43
1:A:1169:VAL:HA	1:A:1170:PRO:HD3	1.76	0.43
1:A:1190:THR:HG21	1:A:1202:LEU:HD21	2.00	0.43
1:B:2027:GLU:C	1:B:2029:PHE:N	2.76	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2202:LEU:C	1:B:2203:VAL:HG13	2.44	0.43
1:B:2386:ILE:HG12	1:B:2416:LEU:HG	2.00	0.43
1:A:1151:ARG:HH11	1:A:1151:ARG:CG	2.32	0.43
1:A:1296:LEU:CD1	1:A:1378:MET:HE1	2.49	0.43
1:A:1380:LEU:HD23	1:A:1380:LEU:HA	1.72	0.43
1:B:2043:LYS:CA	1:B:2065:HIS:CD2	2.87	0.43
1:B:2282:SER:CB	1:B:2362:GLN:HA	2.31	0.43
1:A:1152:TYR:CE2	1:A:1170:PRO:HG3	2.54	0.42
1:A:1269:ASN:ND2	1:A:1283:ALA:CB	2.81	0.42
1:B:2074:LYS:HG2	1:B:2108:HIS:CE1	2.54	0.42
1:B:2161:ASP:OD1	1:B:2161:ASP:N	2.52	0.42
1:B:2311:THR:O	1:B:2312:GLY:C	2.62	0.42
1:B:2383:ARG:N	1:B:2384:PRO:CD	2.81	0.42
1:B:2473:ASP:OD1	1:B:2473:ASP:C	2.60	0.42
1:B:2193:HIS:NE2	1:B:2385:ILE:HD11	2.34	0.42
1:B:2289:THR:O	1:B:2291:GLN:N	2.52	0.42
1:A:1438:ASP:O	1:A:1439:SER:HB2	2.19	0.42
1:B:2275:THR:CG2	1:B:2281:LEU:HD22	2.49	0.42
1:A:1098:ASP:O	1:A:1099:GLY:O	2.38	0.42
1:A:1127:SER:C	1:A:1129:ALA:N	2.74	0.42
1:B:2400:VAL:HG13	1:B:2401:THR:N	2.26	0.42
1:B:2432:TYR:CG	1:B:2448:PRO:HB3	2.54	0.42
1:B:2438:ASP:O	1:B:2439:SER:HB2	2.20	0.42
1:A:1071:ALA:O	1:A:1078:VAL:HA	2.19	0.42
1:A:1407:ASN:ND2	1:A:1476:GLY:HA3	2.35	0.42
1:B:2065:HIS:ND1	1:B:2065:HIS:C	2.78	0.42
1:A:1150:LYS:CG	1:A:1151:ARG:HE	2.21	0.42
1:A:1289:THR:O	1:A:1291:GLN:N	2.52	0.42
1:A:1311:THR:O	1:A:1311:THR:HG22	2.19	0.42
1:B:2127:SER:O	1:B:2128:PRO:C	2.62	0.42
1:B:2400:VAL:HG13	1:B:2401:THR:HG23	2.01	0.42
1:A:1218:SER:C	1:A:1220:LYS:N	2.64	0.42
1:A:1282:SER:HB3	1:A:1362:GLN:CA	2.32	0.42
1:B:2030:GLY:O	1:B:2031:PHE:C	2.63	0.42
1:B:2166:ASP:OD1	1:B:2166:ASP:N	2.52	0.42
1:B:2181:PHE:CD1	1:B:2186:TYR:CE1	3.08	0.42
1:B:2341:ARG:NH1	1:B:2375:LEU:HD11	2.34	0.42
1:A:1266:GLN:HA	1:A:1271:ARG:O	2.20	0.42
1:A:1473:ASP:CG	1:A:1477:VAL:HG22	2.45	0.42
1:B:2041:LYS:H	1:B:2044:GLN:HB2	1.84	0.42
1:B:2078:VAL:HG12	1:B:2120:SER:HA	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1434:THR:HG23	1:A:1449:VAL:CG1	2.48	0.42
1:B:2096:HIS:O	1:B:2098:ASP:N	2.53	0.42
1:B:2158:ARG:HH11	1:B:2158:ARG:H	1.68	0.42
1:B:2486:ASP:OD1	1:B:2486:ASP:C	2.62	0.42
1:A:1102:SER:OG	1:A:1126:VAL:CG1	2.68	0.42
1:A:1342:ASP:HB2	1:A:1452:PHE:CD2	2.55	0.42
1:A:1361:GLY:O	1:A:1362:GLN:O	2.38	0.42
1:A:1432:TYR:CE1	1:A:1448:PRO:HB3	2.55	0.42
1:A:1063:ARG:HG3	1:A:1063:ARG:HH11	1.83	0.41
1:A:1218:SER:O	1:A:1220:LYS:N	2.48	0.41
1:A:1343:ARG:NH2	1:A:1450:ASP:OD2	2.49	0.41
1:A:1454:GLU:OE1	1:A:1464:LYS:HE3	2.20	0.41
1:B:2127:SER:O	1:B:2129:ALA:N	2.52	0.41
1:A:1040:LEU:HD11	1:A:1045:ILE:HG22	2.02	0.41
1:A:1100:ARG:HB3	1:A:1133:SER:HA	2.00	0.41
1:A:1490:LEU:HA	1:A:1490:LEU:HD23	1.76	0.41
1:B:2040:LEU:HD11	1:B:2045:ILE:HG22	2.02	0.41
1:B:2167:ARG:NH2	1:B:2171:TRP:HB3	2.35	0.41
1:B:2437:SER:C	1:B:2439:SER:H	2.27	0.41
1:A:1155:LEU:HD23	1:A:1155:LEU:C	2.43	0.41
1:A:1166:ASP:OD1	1:A:1166:ASP:N	2.52	0.41
1:A:1416:LEU:HA	1:A:1424:ASN:O	2.20	0.41
1:A:1432:TYR:CD1	1:A:1448:PRO:HB3	2.55	0.41
1:B:2160:ALA:O	1:B:2161:ASP:HB2	2.20	0.41
1:B:2359:LYS:HG3	1:B:2360:ASN:H	1.85	0.41
1:A:1029:PHE:HD2	1:A:1029:PHE:HA	1.77	0.41
1:A:1386:ILE:HG12	1:A:1416:LEU:HG	2.01	0.41
1:A:1150:LYS:HG3	1:A:1150:LYS:O	2.18	0.41
1:B:2208:PRO:HG2	1:B:2209:ALA:N	2.35	0.41
1:A:1010:VAL:CG1	1:A:1256:LEU:CB	2.98	0.41
1:A:1177:ILE:CG2	1:A:1188:VAL:HG13	2.51	0.41
1:B:2023:TYR:O	1:B:2024:LEU:C	2.63	0.41
1:B:2048:LEU:CD1	1:B:2060:VAL:HB	2.49	0.41
1:B:2317:LEU:HD12	1:B:2317:LEU:HA	1.68	0.41
1:A:1074:LYS:HG2	1:A:1108:HIS:ND1	2.36	0.41
1:A:1150:LYS:O	1:A:1150:LYS:HE3	2.20	0.41
1:B:2127:SER:C	1:B:2129:ALA:N	2.78	0.41
1:B:2322:GLY:HA2	1:B:2364:ALA:HB2	2.02	0.41
1:B:2367:VAL:HG12	1:B:2368:GLU:N	2.35	0.41
1:B:2470:LEU:HD12	1:B:2470:LEU:HA	1.92	0.41
1:A:1109:ARG:HH11	1:A:1109:ARG:CG	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1205:ARG:NE	1:A:1205:ARG:O	2.54	0.41
1:A:1215:GLU:CD	1:A:1230:TYR:HH	2.27	0.41
1:B:2093:ILE:CG2	1:B:2101:TRP:CE2	3.04	0.41
1:B:2100:ARG:HB3	1:B:2133:SER:HA	2.01	0.41
1:B:2141:GLN:NE2	1:B:2178:THR:HG23	2.36	0.41
1:B:2183:ASP:O	1:B:2185:ARG:N	2.54	0.41
1:B:2444:SER:HB2	1:B:2445:GLY:H	1.67	0.41
1:A:1338:ILE:HG23	1:A:1345:ILE:CD1	2.50	0.41
1:B:2205:ARG:O	1:B:2205:ARG:CG	2.69	0.41
1:B:2361:GLY:O	1:B:2362:GLN:O	2.38	0.41
1:A:1048:LEU:HD11	1:A:1060:VAL:CB	2.51	0.40
1:A:1154:HIS:HE1	1:A:1164:ALA:HB3	1.85	0.40
1:B:2203:VAL:HG21	1:B:2205:ARG:CZ	2.51	0.40
1:A:1152:TYR:CD2	1:A:1170:PRO:HG3	2.56	0.40
1:B:2197:ARG:HD2	1:B:2199:ASP:OD2	2.21	0.40
1:A:1063:ARG:HD3	1:A:1069:TYR:CE2	2.56	0.40
1:A:1197:ARG:HB3	1:A:1199:ASP:OD1	2.21	0.40
1:A:1268:ALA:C	1:A:1270:GLU:N	2.78	0.40
1:B:2304:LYS:HG2	1:B:2337:ASP:OD2	2.20	0.40
1:B:2385:ILE:HG23	1:B:2413:VAL:HG13	2.02	0.40
1:A:1212:TYR:CZ	1:A:1231:LEU:HD21	2.56	0.40
1:A:1346:THR:HG22	1:A:1346:THR:O	2.21	0.40
1:B:2061:CYS:C	1:B:2062:LEU:HD12	2.46	0.40
1:B:2185:ARG:HH22	1:B:2226:CYS:HA	1.86	0.40
1:B:2234:SER:O	1:B:2235:GLY:O	2.39	0.40
1:B:2017:ILE:HG23	1:B:2022:LYS:O	2.22	0.40
1:B:2027:GLU:C	1:B:2029:PHE:H	2.28	0.40
1:B:2404:LEU:HD22	1:B:2442:THR:HA	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1075:ASP:OD1	1:B:2343:ARG:NH1[1_565]	2.15	0.05

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	469/493 (95%)	390 (83%)	61 (13%)	18 (4%)	2	10
1	B	468/493 (95%)	390 (83%)	59 (13%)	19 (4%)	2	9
All	All	937/986 (95%)	780 (83%)	120 (13%)	37 (4%)	2	10

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1029	PHE
1	A	1116	GLU
1	A	1158	ARG
1	A	1160	ALA
1	A	1227	GLU
1	A	1399	LYS
1	A	1445	GLY
1	B	2029	PHE
1	B	2097	ASP
1	B	2116	GLU
1	B	2158	ARG
1	B	2160	ALA
1	B	2227	GLU
1	B	2281	LEU
1	B	2399	LYS
1	B	2445	GLY
1	A	1097	ASP
1	A	1099	GLY
1	A	1235	GLY
1	A	1332	ALA
1	A	1342	ASP
1	A	1362	GLN
1	B	2099	GLY
1	B	2235	GLY
1	B	2343	ARG

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Mol	Chain	Res	Type
1	B	2362	GLN
1	A	1218	SER
1	B	2172	GLY
1	B	2332	ALA
1	B	2342	ASP
1	A	1080	CYS
1	A	1228	GLY
1	A	1367	VAL
1	B	2228	GLY
1	B	2367	VAL
1	B	2218	SER
1	A	1320	THR

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	391/404 (97%)	311 (80%)	80 (20%)	1 4
1	B	391/404 (97%)	307 (78%)	84 (22%)	1 3
All	All	782/808 (97%)	618 (79%)	164 (21%)	1 4

All (164) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1008	GLU
1	A	1010	VAL
1	A	1014	PHE
1	A	1016	LEU
1	A	1024	LEU
1	A	1029	PHE
1	A	1032	LYS
1	A	1038	SER
1	A	1040	LEU
1	A	1047	THR
1	A	1066	LEU

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Mol	Chain	Res	Type
1	A	1074	LYS
1	A	1078	VAL
1	A	1090	ARG
1	A	1100	ARG
1	A	1102	SER
1	A	1103	LEU
1	A	1109	ARG
1	A	1115	THR
1	A	1116	GLU
1	A	1117	ASP
1	A	1126	VAL
1	A	1127	SER
1	A	1130	GLU
1	A	1138	MET
1	A	1140	PRO
1	A	1141	GLN
1	A	1147	VAL
1	A	1148	THR
1	A	1150	LYS
1	A	1151	ARG
1	A	1158	ARG
1	A	1162	GLU
1	A	1168	ASP
1	A	1169	VAL
1	A	1173	VAL
1	A	1178	THR
1	A	1182	GLN
1	A	1189	GLN
1	A	1205	ARG
1	A	1213	THR
1	A	1221	VAL
1	A	1229	ARG
1	A	1231	LEU
1	A	1244	LYS
1	A	1248	VAL
1	A	1271	ARG
1	A	1273	VAL
1	A	1281	LEU
1	A	1301	ASP
1	A	1302	THR
1	A	1303	LYS
1	A	1313	LYS

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Mol	Chain	Res	Type
1	A	1316	THR
1	A	1320	THR
1	A	1326	THR
1	A	1334	CYS
1	A	1343	ARG
1	A	1345	ILE
1	A	1346	THR
1	A	1356	THR
1	A	1372	ASP
1	A	1375	LEU
1	A	1380	LEU
1	A	1385	ILE
1	A	1386	ILE
1	A	1395	ILE
1	A	1397	CYS
1	A	1404	LEU
1	A	1408	ARG
1	A	1415	GLN
1	A	1416	LEU
1	A	1428	SER
1	A	1434	THR
1	A	1435	VAL
1	A	1438	ASP
1	A	1444	SER
1	A	1449	VAL
1	A	1470	LEU
1	A	1471	LYS
1	B	2008	GLU
1	B	2010	VAL
1	B	2016	LEU
1	B	2024	LEU
1	B	2029	PHE
1	B	2032	LYS
1	B	2033	VAL
1	B	2040	LEU
1	B	2047	THR
1	B	2078	VAL
1	B	2090	ARG
1	B	2100	ARG
1	B	2102	SER
1	B	2103	LEU
1	B	2109	ARG

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Mol	Chain	Res	Type
1	B	2116	GLU
1	B	2117	ASP
1	B	2126	VAL
1	B	2127	SER
1	B	2130	GLU
1	B	2138	MET
1	B	2140	PRO
1	B	2141	GLN
1	B	2147	VAL
1	B	2148	THR
1	B	2150	LYS
1	B	2151	ARG
1	B	2158	ARG
1	B	2162	GLU
1	B	2168	ASP
1	B	2169	VAL
1	B	2173	VAL
1	B	2178	THR
1	B	2182	GLN
1	B	2189	GLN
1	B	2205	ARG
1	B	2213	THR
1	B	2221	VAL
1	B	2231	LEU
1	B	2240	LEU
1	B	2244	LYS
1	B	2248	VAL
1	B	2269	ASN
1	B	2271	ARG
1	B	2273	VAL
1	B	2280	ASP
1	B	2281	LEU
1	B	2284	ASN
1	B	2301	ASP
1	B	2302	THR
1	B	2303	LYS
1	B	2310	HIS
1	B	2313	LYS
1	B	2316	THR
1	B	2320	THR
1	B	2326	THR
1	B	2334	CYS

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Mol	Chain	Res	Type
1	B	2343	ARG
1	B	2345	ILE
1	B	2346	THR
1	B	2356	THR
1	B	2360	ASN
1	B	2372	ASP
1	B	2375	LEU
1	B	2380	LEU
1	B	2385	ILE
1	B	2386	ILE
1	B	2389	ARG
1	B	2397	CYS
1	B	2400	VAL
1	B	2404	LEU
1	B	2415	GLN
1	B	2416	LEU
1	B	2425	ILE
1	B	2428	SER
1	B	2429	THR
1	B	2434	THR
1	B	2435	VAL
1	B	2438	ASP
1	B	2444	SER
1	B	2446	ASP
1	B	2449	VAL
1	B	2470	LEU
1	B	2471	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1011	GLN
1	A	1021	ASN
1	A	1124	GLN
1	A	1141	GLN
1	A	1182	GLN
1	A	1324	GLN
1	A	1392	HIS
1	A	1415	GLN
1	B	2011	GLN
1	B	2013	GLN
1	B	2021	ASN

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Mol	Chain	Res	Type
1	B	2124	GLN
1	B	2141	GLN
1	B	2182	GLN
1	B	2189	GLN
1	B	2198	HIS
1	B	2284	ASN
1	B	2324	GLN
1	B	2415	GLN
1	B	2424	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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.