



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:58 PM GMT

PDB ID : 1DFC
Title : CRYSTAL STRUCTURE OF HUMAN FASCIN, AN ACTIN-CROSSLINKING PROTEIN
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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
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

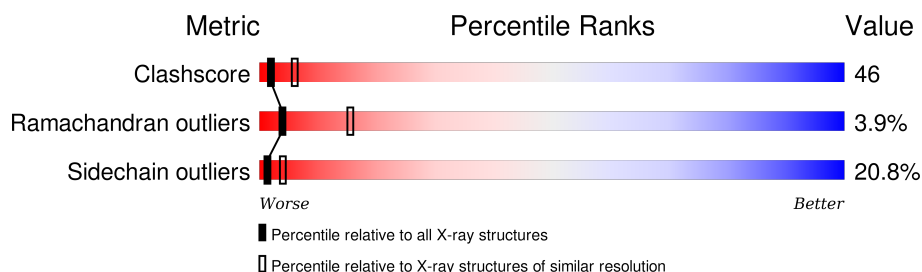
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

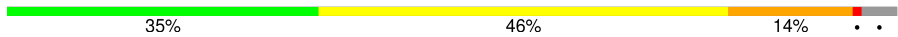
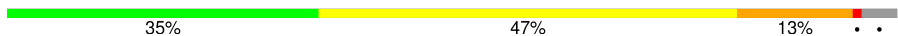
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	493	 35% 46% 14% . .
1	B	493	 35% 47% 13% . .

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
1	A	475	Total	C	N	O	S	0	0	0
			3716	2326	663	714	13			
1	B	474	Total	C	N	O	S	0	0	0
			3711	2323	662	713	13			

S2489	Q2415	R2348	A2383	E2215	Y2145
Y2493	L2416	N2351	N2284	F2216	S2146
	F2418		Q2285	R2217	V2147
	N2419	F2354	E2288	S2218	T2148
	D2420	V2355	T2289	G2219	R2149
	G2421	T2356	D2290	K2220	K2150
	A2422	S2357	Q2291	V2221	R2151
		K2358	E2292		Y2152
	I2425	K2359	T2293	R2224	
	K2426	N2360	F2294	D2225	S2156
	D2427	G2361	Q2295	C2226	A2157
	S2428	Q2362	L2296	E2227	R2158
	T2429	L2363		G2228	P2159
	G2430	A2364	D2299	R2229	A2160
	K2431	A2365	R2300	Y2230	D2161
	Y2432	S2366	D2301	L2231	
	V2433	T2367	T2302	A2232	A2164
	T2434	E2368	K2303	P2233	V2165
		T2369	K2304	S2234	D2166
	D2438	A2370	C2305	G2235	R2167
	S2439	G2371			D2168
		D2372	R2308	G2238	V2169
	T2442		T2309	T2239	P2170
	S2443	L2375	H2310		H2171
	S2444	F2376	T2311	G2243	G2172
	G2445	L2377	G2312	K2244	V2173
	D2446	M2378	K2313		D2174
	T2447	K2379	Y2314	V2248	S2175
	P2448	L2380	V2315		
	V2449	I2381	T2316	D2251	T2178
	D2450	N2382	L2317	E2252	
	F2451	R2383	T2318	L2253	F2181
	F2452	P2384	A2319	F2254	Q2182
	E2454	I2385	T2320	A2255	D2183
	F2455	L2386	G2321	L2256	Q2184
			G2322	E2257	R2185
	C2456		V2323	Q2258	Y2186
	D2457	R2389	Q2324	S2259	S2187
	Y2458	G2390	S2325	C2260	V2188
		E2391	T2326	A2261	Q2189
	K2464	F2394	A2327	Q2262	H2193
	V2465	I2395		V2263	R2194
		G2396	K2330	L2265	
	R2466	C2397	N2331	Q2266	
	Y2469	R2398	A2332		R2197
	L2470	K2399	S2333	N2269	H2198
	K2471	V2400	C2334	E2270	D2199
	G2472	T2401		R2271	
	D2473		D2337	N2272	V2203
	H2474	L2404	I2338	V2273	A2204
	A2475	D2405	E2339	S2274	R2205
	G2476	A2406	M2340	T2275	P2206
	V2477	N2407	R2341	ARG	E2207
		R2408	D2342	GLN	P2208
			R2343	GLY	A2209
	A2482		R2344	MET	T2210
		Y2411	I2345		G2211
	D2486	D2412	T2346	D2280	Y2212
	P2487	V2413	L2347	L2281	T2213
	A2488	F2414		S2282	L2214

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be 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.	Xtriage
Total number of atoms	7427	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	0.96	2/3793 (0.1%)	0.98	3/5126 (0.1%)
1	B	0.95	3/3788 (0.1%)	0.98	2/5119 (0.0%)
All	All	0.96	5/7581 (0.1%)	0.98	5/10245 (0.0%)

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

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

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	2456	CYS	CB-SG	-6.68	1.70	1.82
1	A	1397	CYS	CB-SG	-6.12	1.71	1.82
1	B	2260	CYS	CB-SG	-5.68	1.72	1.81
1	A	1061	CYS	CB-SG	-5.42	1.73	1.81
1	B	2305	CYS	CB-SG	-5.34	1.73	1.81

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1383	ARG	NE-CZ-NH1	-6.77	116.91	120.30
1	B	2194	ARG	NE-CZ-NH1	-6.15	117.22	120.30
1	A	1387	VAL	N-CA-C	-5.67	95.70	111.00
1	A	1363	LEU	CA-CB-CG	5.30	127.50	115.30
1	B	2404	LEU	CA-CB-CG	5.27	127.42	115.30

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	343	1
1	B	3711	0	3597	336	1
All	All	7427	0	7196	679	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 46.

All (679) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:HH11	1:A:1343:ARG:HG3	1.43	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:2205:ARG:HH22	1:B:2207:GLU:CD	1.88	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:A:1205:ARG:HH22	1:A:1207:GLU:CD	1.89	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:O	1:A:1011:GLN:HG3	1.88	0.72
1:A:1205:ARG:HH22	1:A:1207:GLU:CG	2.01	0.72
1:B:2299:ASP:CG	1:B:2302:THR:HG23	2.09	0.72
1:A:1063:ARG:NE	1:A:1067:GLY:HA2	2.04	0.72
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: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: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:HH11	1:B:2343:ARG:HG3	1.56	0.70
1:A:1027:GLU:HB3	1:A:1029:PHE:HB2	1.72	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:1203:VAL:HG21	1:A:1205:ARG:HE	1.57	0.69
1:A:1111:TYR:CE2	1:A:1126:VAL:HG22	2.28	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:O	1:B:2011:GLN:HG3	1.92	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:HB3	1:B:2090:ARG:HH11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2355:VAL:CG1	1:B:2363:LEU:HD13	2.25	0.67
1:B:2094:VAL:HB	1:B:2102:SER:HB3	1.77	0.67
1:B:2165:VAL:HG13	1:B:2165:VAL:O	1.95	0.67
1:B:2391:GLU:OE2	1:B:2487:PRO:HB2	1.93	0.67
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:1299:ASP:CG	1:A:1302:THR:HG23	2.16	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: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:2150:LYS:C	1:B:2151:ARG:HD3	2.16	0.65
1:B:2398:ARG:HA	1:B:2408:ARG:HH12	1.61	0.65
1:A:1218:SER:C	1:A:1220:LYS:H	1.99	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: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:B:2385:ILE:HG23	1:B:2413:VAL:CG1	2.27	0.65
1:A:1339:GLU:HB3	1:A:1346:THR:CG2	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:B:2040:LEU:HD12	1:B:2040:LEU:C	2.17	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:B:2339:GLU:HB3	1:B:2346:THR:HB	1.79	0.63
1:A:1182:GLN:NE2	1:A:1210:THR:OG1	2.31	0.63
1:B:2394:PHE:CG	1:B:2411:TYR:HB3	2.34	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1382:ASN:O	1:A:1383:ARG:HD3	1.98	0.62
1:A:1139:HIS:ND1	1:A:1141:GLN:HG3	2.10	0.62
1:B:2382:ASN:O	1:B:2383:ARG:HD3	2.00	0.62
1:A:1127:SER:N	1:A:1130:GLU:HG2	2.10	0.62
1:B:2316:THR:O	1:B:2323:VAL:HA	2.00	0.62
1:B:2426:LYS:HD3	1:B:2432:TYR:CZ	2.34	0.62
1:A:1425:ILE:HG21	1:A:1433:TRP:CE2	2.33	0.62
1:A:1008:GLU:HG2	1:A:1257:GLU:HB3	1.80	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:A:1042:LYS:O	1:A:1045:ILE:HG12	2.00	0.62
1:A:1122:PHE:O	1:A:1122:PHE:CD1	2.52	0.61
1:A:1426:LYS:HA	1:A:1431:LYS:O	1.99	0.61
1:B:2269:ASN:C	1:B:2269:ASN:OD1	2.38	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:OE2	1:B:2252:GLU:N	2.33	0.61
1:B:2486:ASP:OD1	1:B:2488:ALA:HB3	2.00	0.61
1:B:2294:PHE:HE2	1:B:2309:THR:HG22	1.65	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:1394:PHE:CG	1:A:1411:TYR:HB3	2.36	0.61
1:A:1229:ARG:HG2	1:A:1243:GLY:O	2.01	0.61
1:B:2136:ILE:HD12	1:B:2138:MET:SD	2.41	0.60
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:2386:ILE:CG1	1:B:2416:LEU:HG	2.29	0.60
1:A:1150:LYS:O	1:A:1151:ARG:HD3	2.01	0.60
1:A:1383:ARG:O	1:A:1416:LEU:HD11	2.01	0.60
1:A:1183:ASP:C	1:A:1185:ARG:H	2.05	0.60
1:A:1438:ASP:N	1:A:1438:ASP:OD1	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:1385:ILE:HG23	1:A:1413:VAL:CG1	2.32	0.59
1:A:1215:GLU:OE2	1:A:1230:TYR:OH	2.20	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: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:A:1040:LEU:C	1:A:1040:LEU:HD12	2.23	0.59
1:A:1165:VAL:HG11	1:A:1233:PRO:HB3	1.83	0.59
1:B:2351:ASN:C	1:B:2351:ASN:OD1	2.40	0.59
1:A:1314:TYR:CZ	1:A:1330:LYS:HE2	2.38	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:2465:VAL:HG13	1:B:2465:VAL:O	2.01	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:A:1145:TYR:HB3	1:A:1255:ALA:HB3	1.85	0.59
1:A:1150:LYS:C	1:A:1151:ARG:HD3	2.23	0.58
1:B:2354:PHE:CE2	1:B:2370:ALA:HB2	2.37	0.58
1:A:1404:LEU:HD21	1:A:1433:TRP:CE2	2.38	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:B:2165:VAL:HG12	1:B:2238:GLY:O	2.03	0.58
1:A:1291:GLN:HB2	1:A:1292:GLU:OE1	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:B:2386:ILE:HD11	1:B:2416:LEU:HG	1.86	0.58
1:A:1203:VAL:HG21	1:A:1205:ARG:NE	2.19	0.58
1:A:1386:ILE:CG1	1:A:1416:LEU:HG	2.33	0.58
1:A:1348:ARG:HB2	1:A:1354:PHE:CE1	2.38	0.58
1:B:2266:GLN:HB3	1:B:2377:LEU:HB3	1.85	0.57
1:A:1358:LYS:HB3	1:A:1360:ASN:HD21	1.68	0.57
1:B:2269:ASN:O	1:B:2270:GLU:HB2	2.04	0.57
1:B:2148:THR:HG21	1:B:2251:ASP:CG	2.24	0.57
1:B:2425:ILE:HG21	1:B:2433:TRP:CE2	2.39	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:2348:ARG:HB2	1:B:2354:PHE:CE1	2.39	0.57
1:A:1234:SER:OG	1:A:1241:LYS:HD3	2.04	0.57
1:A:1203:VAL:CB	1:A:1205:ARG:HE	2.17	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2198:HIS:ND1	1:B:2209:ALA:HB1	2.19	0.57
1:B:2218:SER:C	1:B:2220:LYS:H	2.08	0.57
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:B:2324:GLN:CG	1:B:2326:THR:HB	2.35	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:2398:ARG:NH1	1:B:2405:ASP:OD1	2.37	0.56
1:B:2316:THR:N	1:B:2324:GLN:O	2.39	0.56
1:A:1486:ASP:HB2	1:A:1487:PRO:HD2	1.88	0.56
1:A:1049:GLU:OE2	1:A:1063:ARG:HG3	2.05	0.56
1:A:1386:ILE:CD1	1:A:1416:LEU:HG	2.35	0.56
1:A:1269:ASN:HD21	1:A:1283:ALA:CB	2.19	0.56
1:A:1205:ARG:NH2	1:A:1207:GLU:HG2	2.21	0.56
1:B:2422:ALA:HB1	1:B:2450:ASP:HB3	1.88	0.56
1:A:1183:ASP:C	1:A:1185:ARG:N	2.57	0.56
1:A:1090:ARG:HB3	1:A:1090:ARG:HH11	1.70	0.56
1:B:2358:LYS:HB3	1:B:2360:ASN:HD21	1.69	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:B:2203:VAL:HG21	1:B:2205:ARG:NH2	2.20	0.56
1:A:1294:PHE:CE2	1:A:1309:THR:HG22	2.41	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:B:2197:ARG:HD2	1:B:2199:ASP:CG	2.27	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:A:1294:PHE:HE2	1:A:1309:THR:HG22	1.72	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:O	1:B:2188:VAL:HG12	2.05	0.55
1:B:2041:LYS:O	1:B:2045:ILE:HG23	2.06	0.55
1:A:1271:ARG:HH11	1:A:1271:ARG:HG2	1.71	0.55
1:B:2159:PRO:O	1:B:2160:ALA:O	2.25	0.55
1:B:2398:ARG:HA	1:B:2408:ARG:NH1	2.22	0.55
1:B:2063:ARG:NE	1:B:2067:GLY:HA2	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2398:ARG:O	1:B:2400:VAL:N	2.39	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:A:1041:LYS:O	1:A:1045:ILE:HG23	2.07	0.55
1:B:2358:LYS:O	1:B:2359:LYS:C	2.44	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:B:2339:GLU:HB3	1:B:2346:THR:HG22	1.89	0.54
1:A:1315:TRP:O	1:A:1334:CYS:HB3	2.06	0.54
1:B:2416:LEU:CD1	1:B:2416:LEU:N	2.70	0.54
1:A:1180:ALA:HA	1:A:1411:TYR:OH	2.07	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:A:1319:ALA:C	1:A:1321:GLY:H	2.10	0.54
1:A:1203:VAL:HB	1:A:1205:ARG:HE	1.73	0.54
1:A:1422:ALA:HB1	1:A:1450:ASP:HB3	1.90	0.54
1:A:1331:ASN:O	1:A:1333:SER:N	2.42	0.54
1:A:1322:GLY:HA2	1:A:1364:ALA:HB2	1.89	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:2339:GLU:HB3	1:B:2346:THR:CB	2.37	0.53
1:B:2063:ARG:HG2	1:B:2069:TYR:CE1	2.43	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:1151:ARG:N	1:A:1151:ARG:HD3	2.18	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:A:1341:ARG:O	1:A:1342:ASP:C	2.46	0.53
1:B:2049:GLU:OE2	1:B:2063:ARG:HG3	2.09	0.53
1:A:1477:VAL:O	1:A:1477:VAL:HG23	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:A:1304:LYS:HG2	1:A:1337:ASP:OD2	2.09	0.53
1:B:2355:VAL:HG13	1:B:2363:LEU:HD13	1.91	0.53
1:B:2213:THR:OG1	1:B:2224:ARG:HB3	2.09	0.53
1:B:2474:HIS:O	1:B:2475:ALA:CB	2.57	0.53
1:B:2065:HIS:HE1	1:B:2066:LEU:HD21	1.74	0.53
1:A:1185:ARG:NH2	1:A:1226:CYS:HA	2.23	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:B:2238:GLY:O	1:B:2239:THR:C	2.46	0.52
1:A:1136:ILE:HD12	1:A:1138:MET:SD	2.50	0.52
1:A:1229:ARG:HB2	1:A:1229:ARG:CZ	2.39	0.52
1:B:2282:SER:HB3	1:B:2362:GLN:CA	2.29	0.52
1:A:1281:LEU:HD13	1:A:1315:TRP:CE2	2.45	0.52
1:A:1275:THR:HG22	1:A:1281:LEU:HD23	1.92	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:1474:HIS:C	1:A:1476:GLY:H	2.13	0.52
1:B:2346:THR:O	1:B:2346:THR:HG22	2.09	0.52
1:B:2081:GLU:O	1:B:2081:GLU:HG2	2.10	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:2216:PHE:CD1	1:B:2221:VAL:HG23	2.45	0.52
1:A:1331:ASN:O	1:A:1332:ALA:C	2.47	0.52
1:B:2149:ARG:HD2	1:B:2233:PRO:HB2	1.92	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:A:1205:ARG:NH2	1:A:1207:GLU:CG	2.71	0.51
1:B:2010:VAL:CG1	1:B:2256:LEU:O	2.59	0.51
1:A:1358:LYS:HB3	1:A:1360:ASN:ND2	2.25	0.51
1:A:1167:ARG:NH2	1:A:1171:TRP:HB3	2.25	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:B:2342:ASP:O	1:B:2343:ARG:CB	2.57	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:1358:LYS:O	1:A:1359:LYS:C	2.48	0.51
1:A:1201:ARG:HG2	1:A:1202:LEU:H	1.74	0.51
1:B:2205:ARG:NH2	1:B:2207:GLU:HG2	2.26	0.51
1:B:2473:ASP:OD1	1:B:2477:VAL:HG22	2.10	0.51
1:A:1389:ARG:HG2	1:A:1394:PHE:CE2	2.45	0.51
1:B:2183:ASP:C	1:B:2185:ARG:N	2.63	0.51
1:B:2136:ILE:CG2	1:B:2138:MET:SD	2.95	0.51
1:B:2203:VAL:CB	1:B:2205:ARG:HE	2.23	0.51
1:B:2031:PHE:CZ	1:B:2068:ARG:CZ	2.93	0.51
1:B:2474:HIS:C	1:B:2476:GLY:H	2.14	0.51
1:A:1319:ALA:C	1:A:1321:GLY:N	2.64	0.51
1:A:1339:GLU:CB	1:A:1346:THR:HG22	2.41	0.50
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2065:HIS:CE1	1:B:2066:LEU:HD21	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: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:B:2182:GLN:NE2	1:B:2210:THR:OG1	2.44	0.50
1:A:1342:ASP:HB2	1:A:1452:PHE:CG	2.46	0.50
1:A:1238:GLY:O	1:A:1239:THR:C	2.49	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:1154:HIS:CE1	1:A:1164:ALA:HB3	2.47	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:1069:TYR:CD2	1:A:1069:TYR:N	2.78	0.50
1:A:1183:ASP:O	1:A:1185:ARG:N	2.45	0.50
1:A:1082:ARG:HH21	1:A:1086:GLY:HA3	1.77	0.50
1:A:1218:SER:C	1:A:1220:LYS:N	2.64	0.50
1:A:1397:CYS:HB2	1:A:1412:ASP:OD1	2.12	0.50
1:B:2274:SER:HB3	1:B:2292:GLU:HG3	1.94	0.50
1:A:1045:ILE:HD11	1:A:1065:HIS:CD2	2.46	0.50
1:B:2432:TYR:CD1	1:B:2448:PRO:HB3	2.47	0.50
1:A:1197:ARG:HD2	1:A:1199:ASP:CG	2.32	0.50
1:A:1471:LYS:HB2	1:A:1489:SER:HB3	1.93	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:B:2093:ILE:HG21	1:B:2101:TRP:CE2	2.48	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:2205:ARG:HH22	1:B:2207:GLU:HG2	1.76	0.49
1:A:1149:ARG:HD2	1:A:1233:PRO:HB2	1.93	0.49
1:A:1181:PHE:HE1	1:A:1186:TYR:HH	1.58	0.49
1:A:1367:VAL:CG1	1:A:1368:GLU:N	2.76	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:B:2416:LEU:HD13	1:B:2416:LEU:O	2.13	0.49
1:B:2096:HIS:O	1:B:2097:ASP:C	2.50	0.49
1:A:1149:ARG:HD2	1:A:1233:PRO:CB	2.43	0.49
1:B:2486:ASP:HB2	1:B:2487:PRO:HD2	1.94	0.49
1:A:1224:ARG:HG3	1:A:1230:TYR:CE2	2.48	0.49
1:A:1148:THR:HG21	1:A:1251:ASP:OD2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2150:LYS:CG	1:B:2150:LYS:O	2.61	0.49
1:B:2151:ARG:N	1:B:2151:ARG:HD3	2.19	0.49
1:A:1486:ASP:OD1	1:A:1488:ALA:HB3	2.12	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:B:2100:ARG:CB	1:B:2132:TRP:O	2.48	0.48
1:B:2274:SER:CB	1:B:2292:GLU:HG3	2.43	0.48
1:A:1030:GLY:O	1:A:1031:PHE:C	2.51	0.48
1:A:1417:GLU:OE1	1:A:1432:TYR:OH	2.28	0.48
1:B:2275:THR:HG22	1:B:2281:LEU:CD2	2.43	0.48
1:B:2186:TYR:O	1:B:2212:TYR:N	2.44	0.48
1:A:1252:GLU:N	1:A:1252:GLU:OE2	2.47	0.48
1:B:2008:GLU:O	1:B:2258:GLN:HG2	2.13	0.48
1:A:1339:GLU:HB3	1:A:1346:THR:HG22	1.95	0.48
1:A:1149:ARG:NH2	1:A:1235:GLY:O	2.47	0.48
1:B:2342:ASP:HB2	1:B:2452:PHE:CD2	2.49	0.48
1:A:1321:GLY:O	1:A:1364:ALA:HB1	2.14	0.48
1:B:2384:PRO:O	1:B:2385:ILE:HD13	2.14	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:A:1269:ASN:HD21	1:A:1283:ALA:HB3	1.77	0.48
1:B:2203:VAL:HB	1:B:2205:ARG:HE	1.78	0.48
1:B:2063:ARG:HG2	1:B:2069:TYR:CZ	2.49	0.48
1:B:2434:THR:HG23	1:B:2449:VAL:HG11	1.95	0.48
1:A:1022:LYS:HA	1:A:1037:ALA:O	2.13	0.48
1:B:2407:ASN:ND2	1:B:2476:GLY:HA3	2.29	0.48
1:B:2115:THR:HG23	1:B:2116:GLU:N	2.28	0.48
1:A:1261:ALA:HB2	1:A:1493:TYR:CE2	2.49	0.48
1:A:1269:ASN:CG	1:A:1271:ARG:HB2	2.32	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
1:B:2095:ALA:HB2	1:B:2215:GLU:CG	2.36	0.47
1:A:1343:ARG:CG	1:A:1343:ARG:NH1	2.75	0.47
1:A:1215:GLU:OE2	1:A:1230:TYR:CZ	2.67	0.47
1:A:1355:VAL:HG13	1:A:1363:LEU:HD13	1.93	0.47
1:B:2197:ARG:HB3	1:B:2199:ASP:OD1	2.15	0.47
1:A:1373:SER:OG	1:A:1374:GLU:OE2	2.27	0.47
1:A:1351:ASN:C	1:A:1351:ASN:OD1	2.52	0.47
1:A:1158:ARG:HH11	1:A:1158:ARG:H	1.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2313:LYS:HG3	1:B:2327:ALA:O	2.14	0.47
1:B:2017:ILE:HA	1:B:2022:LYS:O	2.14	0.47
1:A:1078:VAL:HG12	1:A:1120:SER:HA	1.96	0.47
1:B:2259:SER:CB	1:B:2383:ARG:HH12	2.28	0.47
1:A:1048:LEU:HD12	1:A:1048:LEU:HA	1.48	0.47
1:B:2385:ILE:CD1	1:B:2415:GLN:HB3	2.44	0.47
1:A:1197:ARG:HA	1:A:1210:THR:HG22	1.95	0.47
1:B:2252:GLU:N	1:B:2252:GLU:CD	2.68	0.47
1:B:2156:SER:HB2	1:B:2164:ALA:HB2	1.95	0.47
1:B:2205:ARG:NH2	1:B:2207:GLU:CG	2.78	0.47
1:A:1339:GLU:OE2	1:A:1346:THR:HG21	2.15	0.47
1:B:2197:ARG:HA	1:B:2210:THR:HG22	1.96	0.47
1:A:1115:THR:O	1:A:1116:GLU:C	2.53	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:A:1132:TRP:N	1:A:1132:TRP:CD1	2.82	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:A:1127:SER:O	1:A:1128:PRO:C	2.53	0.46
1:B:2063:ARG:HE	1:B:2067:GLY:HA2	1.79	0.46
1:B:2109:ARG:CG	1:B:2109:ARG:HH11	2.28	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:B:2093:ILE:HG23	1:B:2101:TRP:CD2	2.51	0.46
1:A:1150:LYS:O	1:A:1150:LYS:CG	2.62	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:1207:GLU:HB2	1:A:1208:PRO:CD	2.42	0.46
1:A:1063:ARG:HG2	1:A:1069:TYR:CE1	2.50	0.46
1:B:2069:TYR:CD2	1:B:2069:TYR:N	2.83	0.46
1:A:1167:ARG:NH1	1:A:1174:ASP:HB2	2.31	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:B:2205:ARG:HH12	1:B:2207:GLU:CB	2.25	0.46
1:A:1010:VAL:HG12	1:A:1256:LEU:C	2.35	0.46
1:A:1030:GLY:O	1:A:1032:LYS:HG2	2.16	0.46
1:A:1008:GLU:CG	1:A:1257:GLU:HB3	2.45	0.46
1:A:1317:LEU:HA	1:A:1317:LEU:HD12	1.59	0.46
1:B:2045:ILE:HG13	1:B:2045:ILE:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1289:THR:C	1:A:1291:GLN:N	2.68	0.46
1:A:1201:ARG:HG2	1:A:1202:LEU:N	2.31	0.46
1:B:2471:LYS:HB2	1:B:2489:SER:HB3	1.98	0.46
1:A:1016:LEU:O	1:A:1023:TYR:HA	2.15	0.46
1:B:2142:VAL:HG21	1:B:2256:LEU:HD22	1.98	0.46
1:A:1473:ASP:OD1	1:A:1474:HIS:O	2.34	0.46
1:B:2465:VAL:CG1	1:B:2465:VAL:O	2.63	0.46
1:B:2048:LEU:HD11	1:B:2060:VAL:CB	2.46	0.46
1:A:1264:VAL:HG21	1:A:1288:GLU:HG2	1.96	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:1340:TRP:HA	1:A:1345:ILE:CD1	2.46	0.45
1:B:2389:ARG:HG3	1:B:2394:PHE:CE2	2.50	0.45
1:B:2379:LYS:HB2	1:B:2418:PHE:CE2	2.51	0.45
1:A:1105:SER:O	1:A:1109:ARG:N	2.45	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:A:1322:GLY:HA2	1:A:1364:ALA:CB	2.46	0.45
1:B:2071:ALA:O	1:B:2078:VAL:HA	2.17	0.45
1:A:1282:SER:CB	1:A:1362:GLN:HA	2.33	0.45
1:A:1187:SER:HB3	1:A:1210:THR:O	2.16	0.45
1:A:1148:THR:HG21	1:A:1251:ASP:CG	2.36	0.45
1:B:2284:ASN:ND2	1:B:2285:GLN:HG2	2.31	0.45
1:A:1111:TYR:CD1	1:A:1111:TYR:N	2.83	0.45
1:B:2031:PHE:CE2	1:B:2068:ARG:NE	2.83	0.45
1:B:2183:ASP:C	1:B:2185:ARG:H	2.18	0.45
1:A:1093:ILE:HD13	1:A:1101:TRP:CH2	2.52	0.45
1:B:2381:ILE:HG13	1:B:2382:ASN:N	2.32	0.45
1:B:2343:ARG:NH2	1:B:2450:ASP:OD2	2.50	0.45
1:A:1398:ARG:CG	1:A:1408:ARG:HH12	2.28	0.45
1:A:1150:LYS:NZ	1:A:1168:ASP:OD1	2.48	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:B:2224:ARG:HG3	1:B:2230:TYR:CE2	2.52	0.45
1:B:2275:THR:CG2	1:B:2281:LEU:CD2	2.94	0.45
1:B:2149:ARG:HD2	1:B:2233:PRO:CB	2.46	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: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:B:2082:ARG:HH21	1:B:2086:GLY:HA3	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2271:ARG:CG	1:B:2271:ARG:HH11	2.30	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:2227:GLU:HB2	1:B:2229:ARG:HE	1.83	0.44
1:B:2065:HIS:CE1	1:B:2066:LEU:CD2	3.01	0.44
1:A:1126:VAL:HA	1:A:1130:GLU:HG3	1.99	0.44
1:B:2095:ALA:HB1	1:B:2224:ARG:HD2	2.00	0.44
1:A:1354:PHE:CD2	1:A:1370:ALA:HA	2.50	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:A:1437:SER:C	1:A:1439:SER:H	2.20	0.44
1:B:2169:VAL:HA	1:B:2170:PRO:HD3	1.82	0.44
1:B:2017:ILE:CG2	1:B:2021:ASN:HA	2.48	0.44
1:B:2263:VAL:HG21	1:B:2378:MET:HE2	1.99	0.44
1:A:1213:THR:OG1	1:A:1224:ARG:HB3	2.17	0.44
1:B:2260:CYS:O	1:B:2261:ALA:C	2.54	0.44
1:A:1139:HIS:ND1	1:A:1140:PRO:HD2	2.33	0.44
1:A:1111:TYR:HD1	1:A:1111:TYR:N	2.16	0.44
1:B:2331:ASN:O	1:B:2332:ALA:C	2.54	0.44
1:B:2338:ILE:HG21	1:B:2340:TRP:CE2	2.52	0.44
1:A:1265:LEU:HB2	1:A:1273:VAL:HG13	1.99	0.44
1:B:2331:ASN:O	1:B:2333:SER:N	2.51	0.44
1:A:1385:ILE:HA	1:A:1385:ILE:HD13	1.66	0.44
1:B:2427:ASP:C	1:B:2427:ASP:OD1	2.55	0.44
1:A:1159:PRO:O	1:A:1160:ALA:C	2.56	0.44
1:B:2361:GLY:C	1:B:2362:GLN:O	2.54	0.44
1:B:2043:LYS:HD2	1:B:2065:HIS:NE2	2.33	0.44
1:B:2426:LYS:HG3	1:B:2431:LYS:O	2.17	0.44
1:A:1319:ALA:O	1:A:1321:GLY:N	2.51	0.44
1:A:1470:LEU:HD12	1:A:1470:LEU:HA	1.75	0.44
1:B:2074:LYS:HG2	1:B:2108:HIS:ND1	2.33	0.44
1:A:1269:ASN:C	1:A:1269:ASN:OD1	2.56	0.43
1:A:1271:ARG:CG	1:A:1271:ARG:HH11	2.29	0.43
1:B:2100:ARG:HB2	1:B:2101:TRP:H	1.45	0.43
1:B:2096:HIS:NE2	1:B:2102:SER:HB2	2.33	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:1017:ILE:HG23	1:A:1022:LYS:O	2.17	0.43
1:B:2269:ASN:CG	1:B:2271:ARG:HB2	2.36	0.43
1:A:1369:THR:O	1:A:1370:ALA:C	2.57	0.43
1:B:2395:ILE:HA	1:B:2405:ASP:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2339:GLU:CB	1:B:2346:THR:CG2	2.94	0.43
1:B:2048:LEU:HD12	1:B:2048:LEU:HA	1.77	0.43
1:A:1361:GLY:C	1:A:1362:GLN:O	2.55	0.43
1:B:2094:VAL:HB	1:B:2102:SER:CB	2.47	0.43
1:B:2343:ARG:HG2	1:B:2452:PHE:HE2	1.82	0.43
1:A:1186:TYR:O	1:A:1212:TYR:N	2.51	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:B:2151:ARG:HA	1:B:2151:ARG:HD3	1.57	0.43
1:A:1190:THR:HG21	1:A:1202:LEU:HD21	2.00	0.43
1:A:1169:VAL:HA	1:A:1170:PRO:HD3	1.76	0.43
1:B:2386:ILE:HG12	1:B:2416:LEU:HG	2.00	0.43
1:B:2282:SER:CB	1:B:2362:GLN:HA	2.31	0.43
1:B:2043:LYS:CA	1:B:2065:HIS:CD2	2.87	0.43
1:A:1151:ARG:HH11	1:A:1151:ARG:CG	2.32	0.43
1:B:2366:SER:O	1:B:2367:VAL:C	2.58	0.43
1:B:2166:ASP:OD1	1:B:2166:ASP:N	2.52	0.43
1:A:1380:LEU:HA	1:A:1380:LEU:HD23	1.72	0.43
1:B:2161:ASP:N	1:B:2161:ASP:OD1	2.52	0.42
1:A:1269:ASN:ND2	1:A:1283:ALA:CB	2.81	0.42
1:B:2383:ARG:N	1:B:2384:PRO:CD	2.81	0.42
1:B:2319:ALA:C	1:B:2321:GLY:H	2.22	0.42
1:B:2074:LYS:HG2	1:B:2108:HIS:CE1	2.54	0.42
1:A:1152:TYR:CE2	1:A:1170:PRO:HG3	2.54	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:B:2382:ASN:CG	1:B:2382:ASN:O	2.57	0.42
1:B:2400:VAL:HG13	1:B:2401:THR:N	2.26	0.42
1:B:2438:ASP:O	1:B:2439:SER:HB2	2.20	0.42
1:B:2432:TYR:CG	1:B:2448:PRO:HB3	2.54	0.42
1:B:2296:LEU:HD13	1:B:2378:MET:HE2	2.01	0.42
1:A:1098:ASP:O	1:A:1099:GLY:O	2.38	0.42
1:A:1407:ASN:ND2	1:A:1476:GLY:HA3	2.35	0.42
1:A:1289:THR:C	1:A:1291:GLN:H	2.21	0.42
1:A:1071:ALA:O	1:A:1078:VAL:HA	2.19	0.42
1:A:1150:LYS:CG	1:A:1151:ARG:HE	2.21	0.42
1:B:2400:VAL:HG13	1:B:2401:THR:HG23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1289:THR:O	1:A:1291:GLN:N	2.52	0.42
1:B:2225:ASP:C	1:B:2225:ASP:OD1	2.57	0.42
1:B:2135:HIS:CD2	1:B:2135:HIS:C	2.93	0.42
1:A:1311:THR:HG22	1:A:1311:THR:O	2.19	0.42
1:A:1282:SER:HB3	1:A:1362:GLN:CA	2.32	0.42
1:B:2181:PHE:CD1	1:B:2186:TYR:CE1	3.08	0.42
1:A:1064:SER:C	1:A:1066:LEU:H	2.23	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: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
1:A:1073:ASP:C	1:A:1073:ASP:OD1	2.58	0.42
1:B:2158:ARG:H	1:B:2158:ARG:HH11	1.68	0.42
1:B:2096:HIS:O	1:B:2098:ASP:N	2.53	0.42
1:B:2289:THR:C	1:B:2291:GLN:N	2.73	0.42
1:B:2343:ARG:C	1:B:2344:ARG:HD2	2.39	0.42
1:A:1434:THR:HG23	1:A:1449:VAL:CG1	2.48	0.42
1:A:1361:GLY:O	1:A:1362:GLN:O	2.38	0.42
1:A:1096:HIS:O	1:A:1097:ASP:C	2.58	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:1432:TYR:CE1	1:A:1448:PRO:HB3	2.55	0.42
1:B:2127:SER:O	1:B:2129:ALA:N	2.52	0.41
1:A:1343:ARG:NH2	1:A:1450:ASP:OD2	2.49	0.41
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:B:2417:GLU:OE1	1:B:2432:TYR:OH	2.26	0.41
1:A:1454:GLU:OE1	1:A:1464:LYS:HE3	2.20	0.41
1:A:1100:ARG:HB3	1:A:1133:SER:HA	2.00	0.41
1:A:1040:LEU:HD11	1:A:1045:ILE:HG22	2.02	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:A:1490:LEU:HD23	1:A:1490:LEU:HA	1.76	0.41
1:A:1416:LEU:HA	1:A:1424:ASN:O	2.20	0.41
1:B:2160:ALA:O	1:B:2161:ASP:HB2	2.20	0.41
1:A:1432:TYR:CD1	1:A:1448:PRO:HB3	2.55	0.41
1:B:2359:LYS:HG3	1:B:2360:ASN:H	1.85	0.41
1:A:1166:ASP:OD1	1:A:1166:ASP:N	2.52	0.41
1:A:1299:ASP:O	1:A:1300:ARG:C	2.59	0.41
1:A:1029:PHE:HA	1:A:1029:PHE:HD2	1.77	0.41
1:A:1386:ILE:HG12	1:A:1416:LEU:HG	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2208:PRO:HG2	1:B:2209:ALA:N	2.35	0.41
1:A:1150:LYS:O	1:A:1150:LYS:HG3	2.18	0.41
1:A:1010:VAL:CG1	1:A:1256:LEU:CB	2.98	0.41
1:B:2048:LEU:CD1	1:B:2060:VAL:HB	2.49	0.41
1:B:2317:LEU:HA	1:B:2317:LEU:HD12	1.68	0.41
1:A:1177:ILE:CG2	1:A:1188:VAL:HG13	2.51	0.41
1:A:1150:LYS:O	1:A:1150:LYS:HE3	2.20	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:1074:LYS:HG2	1:A:1108:HIS:ND1	2.36	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:A:1205:ARG:NE	1:A:1205:ARG:O	2.54	0.41
1:A:1127:SER:C	1:A:1129:ALA:N	2.74	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:A:1109:ARG:HH11	1:A:1109:ARG:CG	2.33	0.41
1:B:2444:SER:HB2	1:B:2445:GLY:H	1.67	0.41
1:B:2361:GLY:O	1:B:2362:GLN:O	2.38	0.41
1:B:2205:ARG:O	1:B:2205:ARG:CG	2.69	0.41
1:A:1338:ILE:HG23	1:A:1345:ILE:CD1	2.50	0.41
1:B:2319:ALA:C	1:B:2321:GLY:N	2.74	0.41
1:B:2024:LEU:C	1:B:2024:LEU:CD2	2.89	0.41
1:B:2203:VAL:HG21	1:B:2205:ARG:CZ	2.51	0.40
1:A:1343:ARG:C	1:A:1344:ARG:HD2	2.38	0.40
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:2284:ASN:C	1:B:2284:ASN:HD22	2.24	0.40
1:B:2141:GLN:C	1:B:2142:VAL:CG1	2.89	0.40
1:B:2218:SER:C	1:B:2220:LYS:N	2.74	0.40
1:B:2173:VAL:O	1:B:2174:ASP:C	2.60	0.40
1:B:2197:ARG:HD2	1:B:2199:ASP:OD2	2.21	0.40
1:A:1152:TYR:CD2	1:A:1170:PRO:HG3	2.56	0.40
1:B:2385:ILE:HG23	1:B:2413:VAL:HG13	2.02	0.40
1:A:1063:ARG:HD3	1:A:1069:TYR:CE2	2.56	0.40
1:A:1346:THR:O	1:A:1346:THR:HG22	2.21	0.40
1:A:1197:ARG:HB3	1:A:1199:ASP:OD1	2.21	0.40
1:B:2304:LYS:HG2	1:B:2337:ASP:OD2	2.20	0.40
1:A:1262:GLN:HB2	1:A:1382:ASN:CG	2.42	0.40
1:A:1314:TYR:HH	1:A:1330:LYS:HE2	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2185:ARG:HH22	1:B:2226:CYS:HA	1.86	0.40
1:A:1212:TYR:CZ	1:A:1231:LEU:HD21	2.56	0.40
1:A:1311:THR:O	1:A:1312:GLY:C	2.58	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: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%)	4	16
1	B	468/493 (95%)	390 (83%)	59 (13%)	19 (4%)	3	14
All	All	937/986 (95%)	780 (83%)	120 (13%)	37 (4%)	4	15

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

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Mol	Chain	Res	Type
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
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 ⓘ

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%)	312 (80%)	79 (20%)	1 4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	391/404 (97%)	307 (78%)	84 (22%)	1	4
All	All	782/808 (97%)	619 (79%)	163 (21%)	1	4

All (163) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
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
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	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	1150	LYS
1	A	1151	ARG
1	A	1158	ARG
1	A	1168	ASP
1	A	1169	VAL
1	A	1171	TRP
1	A	1178	THR
1	A	1182	GLN
1	A	1189	GLN
1	A	1205	ARG
1	A	1213	THR

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Mol	Chain	Res	Type
1	A	1221	VAL
1	A	1229	ARG
1	A	1231	LEU
1	A	1244	LYS
1	A	1248	VAL
1	A	1251	ASP
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	1310	HIS
1	A	1313	LYS
1	A	1316	THR
1	A	1320	THR
1	A	1324	GLN
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	1374	GLU
1	A	1375	LEU
1	A	1380	LEU
1	A	1383	ARG
1	A	1386	ILE
1	A	1389	ARG
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	1438	ASP
1	A	1444	SER
1	A	1446	ASP
1	A	1468	ARG
1	A	1470	LEU

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Mol	Chain	Res	Type
1	A	1471	LYS
1	B	2010	VAL
1	B	2014	PHE
1	B	2016	LEU
1	B	2019	CYS
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
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	2150	LYS
1	B	2151	ARG
1	B	2158	ARG
1	B	2168	ASP
1	B	2169	VAL
1	B	2171	TRP
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	2229	ARG
1	B	2231	LEU
1	B	2244	LYS

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Mol	Chain	Res	Type
1	B	2248	VAL
1	B	2251	ASP
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	2324	GLN
1	B	2326	THR
1	B	2334	CYS
1	B	2343	ARG
1	B	2345	ILE
1	B	2346	THR
1	B	2356	THR
1	B	2372	ASP
1	B	2375	LEU
1	B	2377	LEU
1	B	2380	LEU
1	B	2383	ARG
1	B	2386	ILE
1	B	2389	ARG
1	B	2397	CYS
1	B	2404	LEU
1	B	2408	ARG
1	B	2415	GLN
1	B	2416	LEU
1	B	2428	SER
1	B	2429	THR
1	B	2434	THR
1	B	2438	ASP
1	B	2444	SER
1	B	2446	ASP
1	B	2468	ARG
1	B	2470	LEU

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Mol	Chain	Res	Type
1	B	2471	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1011	GLN
1	A	1021	ASN
1	A	1124	GLN
1	A	1182	GLN
1	A	1324	GLN
1	A	1415	GLN
1	B	2011	GLN
1	B	2013	GLN
1	B	2021	ASN
1	B	2124	GLN
1	B	2141	GLN
1	B	2143	ASN
1	B	2182	GLN
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 carbohydrates 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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

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

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

6.3 Carbohydrates ⓘ

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

6.4 Ligands ⓘ

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

6.5 Other polymers ⓘ

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