



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 08:57 pm GMT

PDB ID : 1QHM
Title : ESCHERICHIA COLI PYRUVATE FORMATE LYASE LARGE DOMAIN
Authors : Leppanen, V.-M.; Merckel, M.C.; Ollis, D.L.; Wong, K.K.; Kozarich, J.W.;
Goldman, A.
Deposited on : 1999-05-19
Resolution : 2.80 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
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

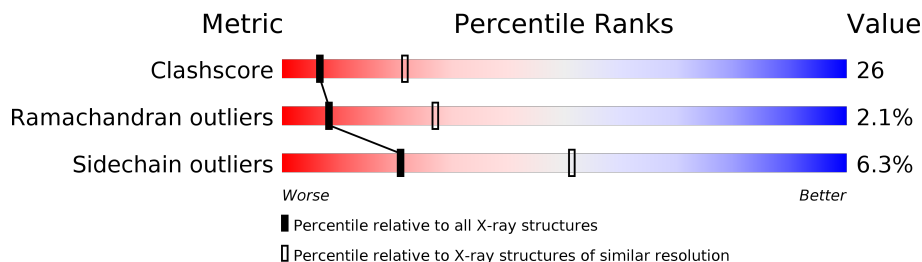
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	112137	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (2.80-2.80)

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	624	 60% 33% 5% •
1	B	624	 58% 35% 5% •

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9810 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 PYRUVATE FORMATE-LYASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	612	Total	C	N	O	S	0	0	1
			4794	3034	810	920	30			
1	B	612	Total	C	N	O	S	0	0	1
			4782	3026	809	917	30			

- Molecule 2 is water.

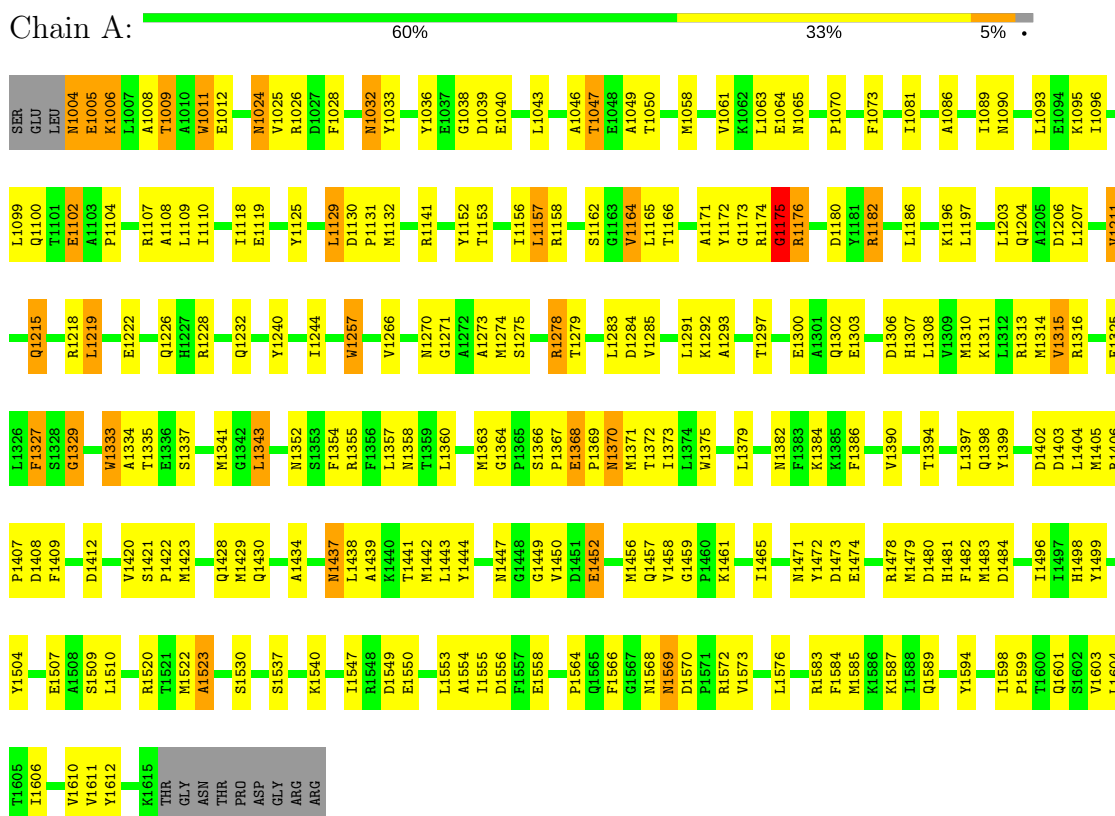
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	125	Total	O	0	0
			125	125		
2	B	109	Total	O	0	0
			109	109		

3 Residue-property plots

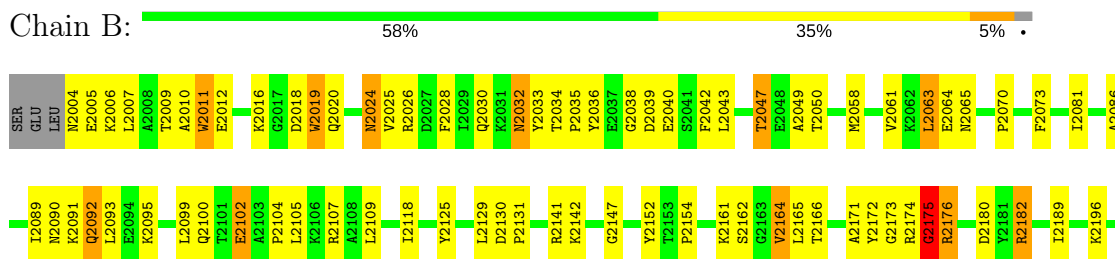
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

Note EDS was not executed.

• Molecule 1: PYRUVATE FORMATE-LYASE



• Molecule 1: PYRUVATE FORMATE-LYASE



A2577	R2478	Y2399	M2314	L2203
R2583	M2479	E2400	V2315	
F2584	D2480	N2401	R2316	D2206
M2585	H2481	D2402		L2207
K2586	F2482	D2403	E2322	
K2587	M2483	L2404		V2211
I2588	D2484	M2405	E2325	
Q2589		R2406	L2326	Q2215
Y2594	I2491	F2407	F2327	
	I2496	D2408	S2328	R2218
Q2601	I2497	F2409	G2329	L2219
S2602	H2498			
V2603	Y2499	D2412	M2333	E2222
L2604			A2334	
	Y2504	V2420	T2335	Q2226
N2609		S2421	E2336	
V2610	E2507	P2422	S2337	K2234
	A2508	M2423		
K2615	S2509	Q2428	M2341	Y2240
THR	L2510	M2429	G2342	
GLY		Q2430	L2343	I2244
ASN	R2520		R2346	
THR		A2434		P2247
PRO	A2523			
ASP	S2535	N2437	K2351	W2257
GLY		L2438	N2352	
ARG	T2539	A2439	S2353	V2266
	K2540	K2440	F2354	
		T2441	R2355	G2271
V2544		M2442	F2356	A2272
K2545		L2443	L2357	A2273
P2546			N2358	M2274
I2547		N2447	I2359	S2275
R2548		G2448	L2360	
D2549				R2278
E2550		D2451	S2366	T2279
	L2553	E2452	P2367	
A2554		K2453	E2368	L2283
I2555	I2555	L2454	P2369	D2284
D2556		K2455	N2370	V2285
F2557	I2556	M2456	M2371	
E2558	D2556	Q2457	T2372	L2291
I2559	F2557	V2458	I2373	K2292
	E2558	G2459	L2374	A2293
		P2460	W2375	
		K2461		T2297
P2564		S2462		
Q2565		E2463	N2382	E2300
F2566	F2566	P2464	F2383	A2301
G2567	G2567	I2465	K2384	Q2302
			K2385	E2303
N2568			F2386	
N2569		D2468		D2306
D2570	N2569	V2469		H2307
P2571	D2570	L2470		L2308
R2572	P2571	N2471	V2390	V2309
V2573	R2572	Y2472		M2310
D2574	V2573	D2473	T2394	K2311
D2575	D2574	E2474		L2312
L2576	L2576			R2313

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	140.80 Å 140.80 Å 215.90 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.80	Depositor
% Data completeness (in resolution range)	99.0 (20.00-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	5.20	Depositor
Refinement program	CNS 0.4	Depositor
R, R_{free}	0.228 , 0.253	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9810	wwPDB-VP
Average B, all atoms (Å ²)	63.0	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	0.46	0/4891	0.66	2/6623 (0.0%)
1	B	0.46	0/4879	0.67	2/6610 (0.0%)
All	All	0.46	0/9770	0.67	4/13233 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1175	GLY	N-CA-C	6.33	128.93	113.10
1	B	2175	GLY	N-CA-C	6.09	128.32	113.10
1	A	1176	ARG	N-CA-C	-5.68	95.66	111.00
1	B	2176	ARG	N-CA-C	-5.52	96.09	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	4794	0	4659	235	0
1	B	4782	0	4636	261	0
2	A	125	0	0	3	0
2	B	109	0	0	5	0
All	All	9810	0	9295	493	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 26.

All (493) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2465:ILE:CA	1:B:2478:ARG:HH12	1.42	1.33
1:B:2465:ILE:CG1	1:B:2478:ARG:NH1	1.96	1.28
1:B:2465:ILE:HG13	1:B:2478:ARG:NH1	1.57	1.14
1:B:2465:ILE:CA	1:B:2478:ARG:NH1	2.11	1.14
1:B:2465:ILE:N	1:B:2478:ARG:HH12	1.49	1.11
1:B:2465:ILE:HA	1:B:2478:ARG:HH12	1.17	1.06
1:B:2465:ILE:HG12	1:B:2478:ARG:CZ	1.85	1.05
1:B:2465:ILE:HA	1:B:2478:ARG:NH1	1.70	1.05
1:B:2465:ILE:HG13	1:B:2478:ARG:HH11	1.09	1.05
1:A:1465:ILE:HA	1:A:1478:ARG:NH2	1.78	0.98
1:B:2016:LYS:HA	1:B:2020:GLN:OE1	1.64	0.96
1:B:2215:GLN:HE21	1:B:2215:GLN:H	1.14	0.94
1:A:1465:ILE:HA	1:A:1478:ARG:HH22	1.29	0.93
1:A:1215:GLN:H	1:A:1215:GLN:HE21	1.11	0.92
1:A:1570:ASP:OD1	1:A:1572:ARG:HG2	1.70	0.91
1:B:2100:GLN:HE22	1:B:2316:ARG:H	1.19	0.88
1:B:2006:LYS:O	1:B:2009:THR:HG22	1.74	0.88
1:A:1284:ASP:HB2	1:A:1352:ASN:HB2	1.54	0.88
1:A:1100:GLN:HE22	1:A:1316:ARG:H	1.21	0.87
1:B:2310:MET:HG2	1:B:2314:MET:HE2	1.56	0.86
1:B:2284:ASP:HB2	1:B:2352:ASN:HB2	1.58	0.85
1:B:2559:ILE:H	1:B:2559:ILE:HD13	1.40	0.84
1:A:1310:MET:HG2	1:A:1314:MET:HE2	1.59	0.83
1:B:2465:ILE:N	1:B:2478:ARG:NH1	2.24	0.83
1:B:2465:ILE:HG12	1:B:2478:ARG:NH1	1.83	0.83
1:B:2465:ILE:HA	1:B:2478:ARG:CZ	2.08	0.82
1:B:2465:ILE:CG1	1:B:2478:ARG:CZ	2.54	0.81
1:A:1011:TRP:CH2	1:A:1186:LEU:O	2.34	0.81
1:A:1447:ASN:ND2	1:A:1554:ALA:H	1.79	0.81
1:B:2032:ASN:N	1:B:2032:ASN:HD22	1.79	0.79
1:B:2196:LYS:HZ2	1:B:2226:GLN:HE22	1.28	0.79
1:A:1447:ASN:HD21	1:A:1554:ALA:H	1.31	0.78
1:A:1004:ASN:HD22	1:A:1006:LYS:H	1.29	0.78
1:A:1465:ILE:N	1:A:1478:ARG:NH1	2.17	0.78
1:B:2100:GLN:NE2	1:B:2315:VAL:HA	1.99	0.78
1:A:1100:GLN:NE2	1:A:1315:VAL:HA	1.99	0.77
1:A:1215:GLN:H	1:A:1215:GLN:NE2	1.82	0.76
1:A:1011:TRP:HH2	1:A:1186:LEU:O	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2465:ILE:CB	1:B:2478:ARG:NH1	2.49	0.75
1:B:2368:GLU:O	1:B:2370:ASN:N	2.20	0.75
1:B:2465:ILE:HA	1:B:2478:ARG:NH2	2.02	0.75
1:A:1368:GLU:O	1:A:1370:ASN:N	2.19	0.73
1:A:1313:ARG:HG2	1:A:1369:PRO:CG	2.19	0.73
1:A:1032:ASN:HD22	1:A:1032:ASN:N	1.85	0.72
1:A:1108:ALA:HB1	2:A:78:HOH:O	1.89	0.72
1:B:2313:ARG:HG2	1:B:2369:PRO:CG	2.20	0.72
1:A:1215:GLN:N	1:A:1215:GLN:HE21	1.88	0.71
1:B:2033:TYR:HA	1:B:2285:VAL:HG12	1.72	0.71
1:B:2215:GLN:H	1:B:2215:GLN:NE2	1.85	0.70
1:B:2573:VAL:HG23	1:B:2574:ASP:N	2.06	0.70
1:A:1033:TYR:HA	1:A:1285:VAL:HG12	1.74	0.69
1:A:1047:THR:HG22	1:A:1050:THR:H	1.58	0.69
1:B:2559:ILE:N	1:B:2559:ILE:HD13	2.07	0.69
1:B:2090:ASN:OD1	1:B:2093:LEU:HD23	1.91	0.69
1:B:2564:PRO:HG2	1:B:2573:VAL:HG13	1.75	0.69
1:A:1465:ILE:HD11	1:A:1478:ARG:HD2	1.73	0.69
1:A:1196:LYS:NZ	1:A:1226:GLN:HE22	1.91	0.68
1:B:2271:GLY:H	1:B:2274:MET:HE1	1.56	0.68
1:A:1090:ASN:HD22	1:A:1093:LEU:H	1.41	0.67
1:B:2369:PRO:O	1:B:2371:MET:HG3	1.94	0.67
1:B:2180:ASP:OD1	1:B:2182:ARG:HD3	1.94	0.67
1:B:2032:ASN:N	1:B:2032:ASN:ND2	2.39	0.67
1:A:1004:ASN:HD22	1:A:1006:LYS:N	1.93	0.67
1:A:1043:LEU:HD21	1:A:1354:PHE:HB3	1.76	0.67
1:B:2372:THR:HG22	1:B:2398:GLN:HB2	1.77	0.67
1:A:1368:GLU:HA	1:A:1368:GLU:OE1	1.94	0.67
1:B:2583:ARG:O	1:B:2587:LYS:HG2	1.95	0.67
1:B:2468:ASP:OD1	1:B:2469:VAL:N	2.28	0.66
1:B:2437:ASN:C	1:B:2437:ASN:HD22	1.99	0.66
1:B:2043:LEU:HD21	1:B:2354:PHE:HB3	1.77	0.66
1:A:1372:THR:HG22	1:A:1398:GLN:HB2	1.78	0.66
1:A:1465:ILE:CD1	1:A:1478:ARG:HD2	2.26	0.66
1:B:2465:ILE:HA	1:B:2478:ARG:HH22	1.61	0.66
1:B:2215:GLN:HE21	1:B:2215:GLN:N	1.92	0.66
1:A:1297:THR:HG23	1:A:1300:GLU:OE1	1.96	0.65
1:B:2368:GLU:HA	1:B:2368:GLU:OE1	1.96	0.65
1:A:1004:ASN:ND2	1:A:1006:LYS:H	1.94	0.65
1:B:2297:THR:HG23	1:B:2300:GLU:OE1	1.96	0.65
1:A:1325:GLU:HA	1:A:1329:GLY:O	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1437:ASN:C	1:A:1437:ASN:HD22	1.99	0.65
1:A:1032:ASN:ND2	1:A:1032:ASN:N	2.45	0.65
1:A:1369:PRO:O	1:A:1371:MET:HG3	1.96	0.65
1:B:2573:VAL:HG23	1:B:2574:ASP:H	1.60	0.64
1:B:2196:LYS:NZ	1:B:2226:GLN:HE22	1.96	0.64
1:A:1271:GLY:H	1:A:1274:MET:HE1	1.61	0.64
1:A:1196:LYS:HZ1	1:A:1226:GLN:HE22	1.44	0.64
1:A:1429:MET:HG2	1:A:1520:ARG:NH1	2.12	0.63
1:A:1583:ARG:O	1:A:1587:LYS:HG2	1.98	0.63
1:B:2203:LEU:HD11	1:B:2219:LEU:HD13	1.80	0.63
1:B:2375:TRP:HA	1:B:2379:LEU:HD11	1.81	0.63
1:A:1109:LEU:HD22	1:A:1118:ILE:HG23	1.80	0.63
1:B:2109:LEU:HD22	1:B:2118:ILE:HG23	1.80	0.63
1:B:2429:MET:HG2	1:B:2520:ARG:NH1	2.13	0.63
1:B:2100:GLN:HE22	1:B:2316:ARG:N	1.95	0.63
1:B:2047:THR:HG22	1:B:2050:THR:H	1.64	0.62
1:A:1601:GLN:OE1	1:A:1603:VAL:HG12	2.00	0.62
1:B:2278:ARG:HG2	1:B:2337:SER:HB2	1.81	0.62
1:A:1089:ILE:HD12	1:A:1310:MET:HE3	1.80	0.62
1:A:1458:VAL:HG23	1:A:1459:GLY:N	2.14	0.62
1:A:1180:ASP:OD1	1:A:1182:ARG:HD3	2.00	0.62
1:A:1465:ILE:HA	1:A:1478:ARG:CZ	1.97	0.62
1:A:1465:ILE:HG13	1:A:1478:ARG:CD	2.21	0.62
1:B:2244:ILE:HG22	1:B:2257:TRP:CE2	2.34	0.62
1:A:1375:TRP:HA	1:A:1379:LEU:HD11	1.82	0.61
1:A:1404:LEU:O	1:A:1408:ASP:HB2	1.99	0.61
1:B:2548:ARG:NH1	2:B:61:HOH:O	2.34	0.61
1:B:2032:ASN:HD22	1:B:2032:ASN:H	1.47	0.61
1:A:1090:ASN:HD22	1:A:1093:LEU:N	1.98	0.61
1:B:2404:LEU:O	1:B:2408:ASP:HB2	2.00	0.61
1:B:2544:VAL:HG12	1:B:2559:ILE:HG22	1.83	0.61
1:A:1437:ASN:ND2	1:A:1439:ALA:H	1.99	0.61
1:B:2311:LYS:HA	1:B:2314:MET:HE3	1.81	0.61
1:A:1244:ILE:HG22	1:A:1257:TRP:CE2	2.37	0.60
1:A:1278:ARG:HG2	1:A:1337:SER:HB2	1.81	0.60
1:A:1313:ARG:HG2	1:A:1369:PRO:CD	2.31	0.60
1:B:2601:GLN:OE1	1:B:2603:VAL:HG12	2.01	0.60
1:A:1279:THR:HG22	1:A:1283:LEU:HG	1.82	0.60
1:A:1311:LYS:HA	1:A:1314:MET:HE3	1.84	0.60
1:A:1047:THR:HG21	1:A:1303:GLU:OE2	2.02	0.60
1:B:2004:ASN:ND2	1:B:2007:LEU:HD13	2.17	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2092:GLN:CD	1:B:2092:GLN:N	2.54	0.60
1:B:2469:VAL:HA	1:B:2544:VAL:O	2.02	0.60
1:A:1090:ASN:ND2	1:A:1093:LEU:HG	2.17	0.59
1:B:2162:SER:OG	1:B:2164:VAL:HG22	2.01	0.59
1:B:2313:ARG:HG2	1:B:2369:PRO:CD	2.32	0.59
1:B:2089:ILE:HD12	1:B:2310:MET:HE3	1.84	0.59
1:B:2313:ARG:HG2	1:B:2369:PRO:HG2	1.85	0.59
1:A:1100:GLN:HE22	1:A:1316:ARG:N	1.97	0.59
1:A:1313:ARG:HG2	1:A:1369:PRO:HG2	1.84	0.59
1:A:1310:MET:HG2	1:A:1314:MET:CE	2.32	0.59
1:A:1175:GLY:O	1:A:1176:ARG:HD2	2.03	0.59
1:B:2279:THR:HG22	1:B:2283:LEU:HG	1.83	0.59
1:B:2604:LEU:C	1:B:2604:LEU:HD23	2.21	0.59
1:B:2302:GLN:NE2	1:B:2355:ARG:HA	2.18	0.58
1:B:2585:MET:O	1:B:2589:GLN:HG3	2.02	0.58
1:A:1564:PRO:HG3	1:A:1572:ARG:HG3	1.86	0.58
1:A:1549:ASP:HB3	1:A:1555:ILE:HG13	1.83	0.58
1:B:2036:TYR:CZ	1:B:2038:GLY:HA3	2.38	0.58
1:B:2437:ASN:ND2	1:B:2439:ALA:H	2.00	0.58
1:B:2175:GLY:O	1:B:2176:ARG:HD2	2.03	0.58
1:B:2465:ILE:HG12	1:B:2478:ARG:NE	2.18	0.58
1:A:1158:ARG:HG2	1:A:1456:MET:HE3	1.86	0.58
1:A:1207:LEU:HD21	1:B:2496:ILE:HD11	1.84	0.58
1:B:2310:MET:HG2	1:B:2314:MET:CE	2.32	0.58
1:B:2402:ASP:CG	1:B:2406:ARG:NH1	2.57	0.58
1:A:1162:SER:OG	1:A:1164:VAL:HG22	2.04	0.58
1:A:1274:MET:HB2	2:A:222:HOH:O	2.04	0.58
1:A:1302:GLN:NE2	1:A:1355:ARG:HA	2.19	0.57
1:A:1402:ASP:CG	1:A:1406:ARG:NH1	2.57	0.57
1:A:1423:MET:HE2	1:A:1428:GLN:O	2.03	0.57
1:A:1465:ILE:CG1	1:A:1478:ARG:CD	2.81	0.57
1:A:1604:LEU:HD23	1:A:1604:LEU:C	2.25	0.57
1:B:2092:GLN:OE1	1:B:2093:LEU:N	2.36	0.57
1:A:1203:LEU:HD11	1:A:1219:LEU:HD13	1.84	0.57
1:A:1611:VAL:HG12	1:A:1612:TYR:N	2.17	0.57
1:A:1484:ASP:OD1	1:A:1587:LYS:HD2	2.04	0.57
1:A:1040:GLU:N	1:A:1040:GLU:OE1	2.36	0.57
1:A:1555:ILE:O	1:A:1556:ASP:HB2	2.03	0.57
1:B:2047:THR:HG21	1:B:2303:GLU:OE2	2.05	0.57
1:A:1585:MET:O	1:A:1589:GLN:HG3	2.04	0.56
1:B:2086:ALA:HA	1:B:2240:TYR:CZ	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2470:LEU:HG	1:B:2546:PRO:HG3	1.87	0.56
1:A:1206:ASP:HA	1:A:1211:VAL:HG13	1.88	0.56
1:B:2437:ASN:HD21	1:B:2439:ALA:HB3	1.70	0.56
1:B:2447:ASN:HD21	1:B:2554:ALA:H	1.51	0.56
1:B:2464:PRO:C	1:B:2478:ARG:HH12	2.08	0.56
1:A:1507:GLU:HB3	1:A:1510:LEU:HD13	1.87	0.56
1:B:2196:LYS:HZ2	1:B:2226:GLN:NE2	2.01	0.56
1:B:2058:MET:HE2	1:B:2058:MET:HA	1.88	0.56
1:B:2448:GLY:HA2	1:B:2462:SER:OG	2.06	0.56
1:B:2459:GLY:HA3	1:B:2482:PHE:CZ	2.40	0.56
1:A:1086:ALA:HA	1:A:1240:TYR:CZ	2.41	0.55
1:B:2484:ASP:OD1	1:B:2587:LYS:HD2	2.05	0.55
1:A:1047:THR:CG2	1:A:1049:ALA:H	2.19	0.55
1:A:1043:LEU:HD12	1:A:1358:ASN:OD1	2.07	0.55
1:B:2070:PRO:HD3	1:B:2125:TYR:CE1	2.42	0.55
1:A:1171:ALA:O	1:A:1172:TYR:HB3	2.06	0.55
1:B:2271:GLY:H	1:B:2274:MET:CE	2.19	0.55
1:B:2102:GLU:H	1:B:2102:GLU:CD	2.10	0.55
1:A:1032:ASN:HD22	1:A:1032:ASN:H	1.54	0.55
1:A:1564:PRO:HB2	1:A:1573:VAL:CG2	2.36	0.55
1:B:2333:TRP:O	1:B:2335:THR:N	2.40	0.55
1:A:1070:PRO:HD3	1:A:1125:TYR:CE1	2.42	0.54
1:A:1420:VAL:HG22	1:A:1430:GLN:OE1	2.08	0.54
1:A:1004:ASN:HD22	1:A:1005:GLU:N	2.06	0.54
1:A:1036:TYR:CZ	1:A:1038:GLY:HA3	2.43	0.54
1:B:2206:ASP:HA	1:B:2211:VAL:HG13	1.88	0.54
1:B:2368:GLU:C	1:B:2370:ASN:N	2.61	0.54
1:A:1089:ILE:CD1	1:A:1310:MET:HE3	2.37	0.54
1:A:1176:ARG:HG3	1:A:1273:ALA:HB3	1.90	0.54
1:A:1333:TRP:O	1:A:1335:THR:N	2.41	0.54
1:A:1373:ILE:HD12	1:A:1399:TYR:CE2	2.43	0.54
1:B:2421:SER:HB2	1:B:2430:GLN:HE22	1.73	0.54
1:A:1102:GLU:H	1:A:1102:GLU:CD	2.10	0.54
1:A:1352:ASN:HA	1:A:1355:ARG:HH11	1.73	0.54
1:B:2058:MET:HA	1:B:2058:MET:CE	2.37	0.54
1:B:2176:ARG:HG3	1:B:2273:ALA:HB3	1.89	0.54
1:B:2539:ILE:HA	1:B:2544:VAL:HG21	1.89	0.54
1:B:2314:MET:HB3	2:B:28:HOH:O	2.06	0.53
1:B:2043:LEU:HD12	1:B:2358:ASN:OD1	2.08	0.53
1:B:2166:THR:O	1:B:2434:ALA:HB1	2.07	0.53
1:B:2507:GLU:HB3	1:B:2510:LEU:HD13	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2423:MET:HE2	1:B:2428:GLN:O	2.07	0.53
1:A:1465:ILE:CG1	1:A:1478:ARG:HD2	2.38	0.53
1:B:2042:PHE:CE2	1:B:2351:LYS:HD2	2.43	0.53
1:B:2047:THR:CG2	1:B:2049:ALA:H	2.21	0.53
1:B:2047:THR:HG22	1:B:2049:ALA:N	2.23	0.53
1:A:1421:SER:HB2	1:A:1430:GLN:HE22	1.73	0.53
1:B:2352:ASN:HA	1:B:2355:ARG:HH11	1.72	0.53
1:B:2386:PHE:O	1:B:2390:VAL:HG23	2.09	0.53
1:B:2570:ASP:O	1:B:2573:VAL:HG22	2.08	0.53
1:A:1291:LEU:C	1:A:1293:ALA:H	2.13	0.53
1:B:2325:GLU:HA	1:B:2329:GLY:O	2.09	0.53
1:A:1004:ASN:ND2	1:A:1005:GLU:H	2.07	0.53
1:A:1058:MET:HA	1:A:1058:MET:CE	2.39	0.52
1:B:2040:GLU:N	1:B:2040:GLU:OE1	2.35	0.52
1:B:2092:GLN:H	1:B:2092:GLN:CD	2.13	0.52
1:B:2372:THR:HA	1:B:2398:GLN:HB2	1.91	0.52
1:A:1357:LEU:HD22	1:A:1397:LEU:HD11	1.91	0.52
1:A:1465:ILE:HG13	1:A:1478:ARG:HD2	1.91	0.52
1:A:1204:GLN:NE2	1:B:2154:PRO:HD2	2.24	0.52
1:B:2171:ALA:O	1:B:2172:TYR:HB3	2.08	0.52
1:B:2244:ILE:HG22	1:B:2257:TRP:CD2	2.45	0.52
1:A:1368:GLU:C	1:A:1370:ASN:N	2.61	0.52
1:A:1047:THR:HG22	1:A:1049:ALA:N	2.24	0.52
1:B:2090:ASN:ND2	1:B:2092:GLN:HE22	2.08	0.52
1:B:2437:ASN:HD22	1:B:2439:ALA:H	1.58	0.52
1:A:1004:ASN:ND2	1:A:1005:GLU:N	2.58	0.51
1:A:1109:LEU:HD22	1:A:1118:ILE:CG2	2.40	0.51
1:A:1442:MET:HG3	1:A:1479:MET:HE2	1.92	0.51
1:B:2373:ILE:HD12	1:B:2399:TYR:CE2	2.45	0.51
1:A:1064:GLU:OE1	1:A:1316:ARG:NH1	2.43	0.51
1:A:1166:THR:O	1:A:1434:ALA:HB1	2.10	0.51
1:B:2564:PRO:HG3	1:B:2572:ARG:HG2	1.91	0.51
1:A:1271:GLY:H	1:A:1274:MET:CE	2.23	0.51
1:A:1279:THR:HG22	1:A:1283:LEU:CD1	2.41	0.51
1:A:1375:TRP:CZ2	1:A:1384:LYS:HD2	2.46	0.51
1:B:2036:TYR:CE1	1:B:2038:GLY:HA3	2.45	0.51
1:B:2341:MET:O	1:B:2406:ARG:HD3	2.11	0.51
1:B:2090:ASN:ND2	1:B:2092:GLN:NE2	2.57	0.51
1:A:1402:ASP:OD2	1:A:1406:ARG:NH1	2.43	0.51
1:B:2402:ASP:OD2	1:B:2406:ARG:NH1	2.44	0.50
1:A:1568:ASN:O	1:A:1570:ASP:N	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2284:ASP:HB2	1:B:2352:ASN:CB	2.36	0.50
1:A:1402:ASP:OD1	1:A:1406:ARG:HB2	2.12	0.50
1:B:2058:MET:HE2	1:B:2061:VAL:HB	1.93	0.50
1:B:2375:TRP:CZ2	1:B:2384:LYS:HD2	2.47	0.50
1:A:1009:THR:O	1:A:1012:GLU:HB2	2.11	0.50
1:A:1437:ASN:HD21	1:A:1439:ALA:HB3	1.76	0.50
1:B:2009:THR:O	1:B:2012:GLU:HG3	2.12	0.50
1:A:1372:THR:HA	1:A:1398:GLN:HB2	1.94	0.50
1:A:1386:PHE:O	1:A:1390:VAL:HG23	2.12	0.50
1:B:2373:ILE:HD11	1:B:2397:LEU:HD13	1.93	0.50
1:B:2402:ASP:OD1	1:B:2406:ARG:HB2	2.12	0.50
1:B:2420:VAL:HG22	1:B:2430:GLN:OE1	2.11	0.50
1:B:2109:LEU:HD22	1:B:2118:ILE:CG2	2.41	0.49
1:A:1058:MET:HE1	1:A:1061:VAL:CB	2.43	0.49
1:A:1099:LEU:HD11	1:A:1104:PRO:HG3	1.93	0.49
1:A:1284:ASP:HB2	1:A:1352:ASN:CB	2.33	0.49
1:B:2086:ALA:HA	1:B:2240:TYR:CE1	2.47	0.49
1:A:1437:ASN:HD22	1:A:1439:ALA:H	1.59	0.49
1:B:2099:LEU:HD11	1:B:2104:PRO:HG3	1.94	0.49
1:B:2544:VAL:HA	1:B:2558:GLU:O	2.12	0.49
1:A:1458:VAL:CG2	1:A:1459:GLY:N	2.75	0.49
1:B:2368:GLU:C	1:B:2370:ASN:H	2.13	0.49
1:A:1058:MET:HE1	1:A:1061:VAL:HB	1.95	0.49
1:B:2423:MET:HE1	1:B:2430:GLN:N	2.28	0.49
1:B:2442:MET:HG3	1:B:2479:MET:HE2	1.93	0.49
1:A:1215:GLN:N	1:A:1215:GLN:NE2	2.55	0.49
1:A:1373:ILE:HD11	1:A:1397:LEU:HD13	1.95	0.49
1:B:2559:ILE:N	1:B:2559:ILE:CD1	2.74	0.49
1:B:2573:VAL:CG2	1:B:2574:ASP:N	2.74	0.49
1:A:1423:MET:HE1	1:A:1430:GLN:N	2.27	0.49
1:B:2604:LEU:HD23	1:B:2604:LEU:O	2.13	0.49
1:A:1090:ASN:CG	1:A:1093:LEU:HD12	2.32	0.48
1:A:1610:VAL:O	1:A:1610:VAL:HG23	2.13	0.48
1:B:2465:ILE:CG1	1:B:2478:ARG:HD2	2.43	0.48
1:B:2039:ASP:HB2	1:B:2040:GLU:OE1	2.13	0.48
1:A:1047:THR:HG22	1:A:1049:ALA:H	1.79	0.48
1:A:1291:LEU:O	1:A:1293:ALA:N	2.46	0.48
1:B:2016:LYS:HA	1:B:2020:GLN:CD	2.30	0.48
1:A:1218:ARG:O	1:A:1222:GLU:HG3	2.14	0.48
1:A:1036:TYR:CE1	1:A:1038:GLY:HA3	2.49	0.48
1:B:2042:PHE:CZ	1:B:2351:LYS:HD2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2549:ASP:O	1:B:2550:GLU:C	2.52	0.48
1:A:1244:ILE:HG22	1:A:1257:TRP:CD2	2.48	0.48
1:B:2279:THR:HG22	1:B:2283:LEU:CD1	2.43	0.48
1:B:2452:GLU:C	1:B:2454:LEU:H	2.17	0.48
1:A:1028:PHE:CE2	1:A:1285:VAL:HG21	2.48	0.48
1:A:1403:ASP:OD1	1:A:1406:ARG:NH2	2.46	0.48
1:A:1073:PHE:HA	1:A:1107:ARG:O	2.13	0.47
1:A:1444:TYR:CD2	1:A:1458:VAL:HG21	2.49	0.47
1:B:2009:THR:HG23	1:B:2010:ALA:N	2.29	0.47
1:B:2028:PHE:CE2	1:B:2285:VAL:HG21	2.49	0.47
1:B:2064:GLU:OE1	1:B:2316:ARG:NH1	2.47	0.47
1:B:2357:LEU:HD22	1:B:2397:LEU:HD11	1.95	0.47
1:A:1472:TYR:HB2	1:A:1540:LYS:HB3	1.97	0.47
1:B:2370:ASN:OD1	1:B:2398:GLN:HG3	2.13	0.47
1:B:2061:VAL:HG12	1:B:2065:ASN:HD21	1.79	0.47
1:A:1211:VAL:O	1:A:1211:VAL:HG22	2.15	0.47
1:A:1343:LEU:HD22	1:A:1412:ASP:OD2	2.15	0.47
1:A:1429:MET:O	1:A:1520:ARG:HA	2.15	0.47
1:B:2073:PHE:HA	1:B:2107:ARG:O	2.13	0.47
1:B:2468:ASP:O	1:B:2469:VAL:HB	2.13	0.47
1:B:2573:VAL:CG2	1:B:2574:ASP:H	2.26	0.47
1:A:1086:ALA:HA	1:A:1240:TYR:CE1	2.49	0.47
1:A:1564:PRO:HG2	1:A:1573:VAL:HG22	1.96	0.47
1:B:2026:ARG:NH2	1:B:2343:LEU:HD23	2.30	0.47
1:A:1039:ASP:HB2	1:A:1040:GLU:OE1	2.14	0.47
1:A:1409:PHE:CZ	1:A:1422:PRO:HB2	2.50	0.47
1:B:2047:THR:HG22	1:B:2049:ALA:H	1.78	0.47
1:B:2090:ASN:OD1	1:B:2093:LEU:CD2	2.60	0.47
1:B:2275:SER:HA	1:B:2335:THR:H	1.79	0.47
1:B:2564:PRO:O	1:B:2573:VAL:HG11	2.15	0.47
1:B:2610:VAL:O	1:B:2610:VAL:HG23	2.15	0.47
1:A:1370:ASN:OD1	1:A:1398:GLN:HG3	2.15	0.46
1:A:1547:ILE:HD11	1:A:1558:GLU:HG3	1.96	0.46
1:B:2092:GLN:OE1	1:B:2092:GLN:N	2.48	0.46
1:B:2081:ILE:HD11	1:B:2509:SER:HB3	1.97	0.46
1:B:2564:PRO:CG	1:B:2573:VAL:HG13	2.43	0.46
1:B:2030:GLN:HE21	1:B:2346:ARG:HH21	1.63	0.46
1:A:1081:ILE:HD11	1:A:1509:SER:HB3	1.96	0.46
1:A:1026:ARG:NH2	1:A:1343:LEU:HD23	2.29	0.46
1:A:1452:GLU:HG3	1:A:1555:ILE:HD13	1.97	0.46
1:B:2058:MET:HE2	1:B:2061:VAL:HG21	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2089:ILE:CD1	1:B:2310:MET:HE3	2.44	0.46
1:B:2556:ASP:OD1	1:B:2557:PHE:N	2.45	0.46
1:B:2406:ARG:HB3	1:B:2407:PRO:CD	2.46	0.46
1:B:2483:MET:CE	1:B:2584:PHE:HB2	2.45	0.46
1:A:1196:LYS:NZ	1:A:1226:GLN:NE2	2.62	0.46
1:A:1530:SER:HB2	1:A:1566:PHE:CD2	2.50	0.46
1:B:2011:TRP:HZ3	1:B:2247:PRO:CB	2.29	0.46
1:B:2472:TYR:HB2	1:B:2540:LYS:HB3	1.98	0.46
1:A:1611:VAL:CG1	1:A:1612:TYR:N	2.78	0.46
1:B:2058:MET:HE2	1:B:2061:VAL:CG2	2.45	0.46
1:B:2141:ARG:NH2	1:B:2504:TYR:O	2.48	0.46
1:A:1341:MET:O	1:A:1406:ARG:HD3	2.16	0.46
1:A:1360:LEU:HB3	1:A:1394:THR:HG21	1.96	0.46
1:A:1058:MET:HE1	1:A:1061:VAL:HG21	1.96	0.46
1:B:2189:ILE:HG21	1:B:2234:LYS:HG3	1.97	0.46
1:B:2360:LEU:HB3	1:B:2394:THR:HG21	1.97	0.46
1:B:2372:THR:HG22	1:B:2398:GLN:CB	2.45	0.46
1:B:2437:ASN:ND2	1:B:2437:ASN:C	2.69	0.46
1:B:2481:HIS:O	1:B:2484:ASP:HB2	2.16	0.46
1:B:2565:GLN:O	1:B:2573:VAL:HG21	2.15	0.46
1:A:1457:GLN:OE1	1:A:1461:LYS:HA	2.15	0.45
1:B:2011:TRP:HZ3	1:B:2247:PRO:CG	2.28	0.45
1:B:2215:GLN:N	1:B:2215:GLN:NE2	2.59	0.45
1:B:2403:ASP:HA	1:B:2406:ARG:NH2	2.31	0.45
1:B:2343:LEU:HD22	1:B:2412:ASP:OD2	2.15	0.45
1:A:1174:ARG:HH11	1:A:1498:HIS:HD2	1.64	0.45
1:A:1275:SER:HA	1:A:1335:THR:H	1.80	0.45
1:B:2373:ILE:N	1:B:2398:GLN:O	2.41	0.45
1:A:1450:VAL:HG11	1:A:1553:LEU:CD1	2.47	0.45
1:A:1437:ASN:HD22	1:A:1438:LEU:N	2.13	0.45
1:B:2222:GLU:O	1:B:2226:GLN:HG3	2.16	0.45
1:B:2429:MET:O	1:B:2520:ARG:HA	2.15	0.45
1:A:1005:GLU:O	1:A:1008:ALA:HB3	2.17	0.45
1:A:1130:ASP:OD1	1:A:1131:PRO:HD2	2.17	0.45
1:B:2266:VAL:O	1:B:2266:VAL:HG12	2.17	0.45
1:B:2564:PRO:HG3	1:B:2572:ARG:CG	2.47	0.45
1:A:1141:ARG:NH2	1:A:1504:TYR:O	2.50	0.45
1:B:2402:ASP:CG	1:B:2406:ARG:HH12	2.20	0.45
1:B:2409:PHE:CZ	1:B:2422:PRO:HB2	2.52	0.45
1:B:2539:ILE:HA	1:B:2544:VAL:CG2	2.46	0.45
1:A:1095:LYS:H	1:A:1307:HIS:CD2	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2130:ASP:OD1	1:B:2131:PRO:HD2	2.17	0.45
1:B:2366:SER:HA	1:B:2367:PRO:HD3	1.84	0.45
1:B:2554:ALA:HB1	1:B:2557:PHE:CZ	2.51	0.45
1:B:2564:PRO:HG2	1:B:2573:VAL:CG1	2.44	0.45
1:A:1402:ASP:CG	1:A:1406:ARG:HH12	2.19	0.44
1:A:1430:GLN:HG2	1:A:1523:ALA:HB2	1.98	0.44
1:A:1420:VAL:HG23	1:A:1523:ALA:HB1	1.98	0.44
1:B:2471:ASN:HD22	1:B:2474:GLU:HB2	1.82	0.44
1:A:1372:THR:HG22	1:A:1398:GLN:CB	2.46	0.44
1:B:2040:GLU:O	1:B:2043:LEU:HB2	2.18	0.44
1:B:2441:THR:HG23	1:B:2482:PHE:HD2	1.82	0.44
1:A:1573:VAL:O	1:A:1576:LEU:HB2	2.17	0.44
1:A:1604:LEU:HD23	1:A:1604:LEU:O	2.18	0.44
1:A:1266:VAL:HG12	1:A:1266:VAL:O	2.16	0.44
1:B:2092:GLN:OE1	1:B:2093:LEU:HD23	2.18	0.44
1:B:2457:GLN:CD	1:B:2461:LYS:HG2	2.38	0.44
1:A:1279:THR:HG22	1:A:1283:LEU:CG	2.45	0.44
1:A:1406:ARG:HB3	1:A:1407:PRO:CD	2.47	0.44
1:B:2058:MET:CE	1:B:2061:VAL:HG21	2.47	0.44
1:A:1510:LEU:N	1:A:1510:LEU:HD12	2.33	0.44
1:A:1549:ASP:HB3	1:A:1555:ILE:CG1	2.48	0.44
1:A:1222:GLU:O	1:A:1226:GLN:HG3	2.17	0.44
1:A:1311:LYS:HD3	1:A:1314:MET:HE1	2.00	0.44
1:A:1569:ASN:CG	2:A:151:HOH:O	2.55	0.44
1:B:2291:LEU:C	1:B:2293:ALA:H	2.21	0.44
1:B:2161:LYS:HG2	1:B:2456:MET:CE	2.48	0.44
1:A:1403:ASP:HA	1:A:1406:ARG:NH2	2.33	0.43
1:B:2011:TRP:CZ3	1:B:2247:PRO:HG3	2.53	0.43
1:A:1090:ASN:ND2	1:A:1093:LEU:CG	2.81	0.43
1:A:1405:MET:O	1:A:1406:ARG:C	2.57	0.43
1:B:2372:THR:HA	1:B:2398:GLN:O	2.18	0.43
1:B:2430:GLN:HG2	1:B:2523:ALA:HB2	2.00	0.43
1:A:1406:ARG:N	1:A:1407:PRO:HD2	2.34	0.43
1:B:2548:ARG:HA	1:B:2553:LEU:O	2.19	0.43
1:A:1360:LEU:HA	1:A:1364:GLY:O	2.19	0.43
1:A:1368:GLU:C	1:A:1370:ASN:H	2.14	0.43
1:B:2058:MET:HE2	1:B:2061:VAL:CB	2.49	0.43
1:A:1174:ARG:HG3	1:A:1175:GLY:N	2.34	0.43
1:A:1313:ARG:HG2	1:A:1369:PRO:HD3	2.01	0.43
1:A:1471:ASN:HD22	1:A:1474:GLU:HB2	1.84	0.43
1:B:2011:TRP:HZ3	1:B:2247:PRO:HB2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2211:VAL:HG22	1:B:2211:VAL:O	2.18	0.43
1:B:2095:LYS:H	1:B:2307:HIS:CD2	2.36	0.43
1:B:2335:THR:OG1	1:B:2370:ASN:ND2	2.51	0.43
1:B:2459:GLY:HA3	1:B:2482:PHE:HZ	1.84	0.43
1:B:2420:VAL:HG23	1:B:2523:ALA:HB1	2.00	0.43
1:A:1437:ASN:C	1:A:1437:ASN:ND2	2.68	0.43
1:B:2403:ASP:OD1	1:B:2406:ARG:NH2	2.47	0.43
1:A:1327:PHE:C	1:A:1329:GLY:N	2.72	0.43
1:A:1441:THR:HG23	1:A:1482:PHE:HD2	1.84	0.43
1:A:1481:HIS:O	1:A:1484:ASP:HB2	2.19	0.43
1:B:2025:VAL:O	1:B:2028:PHE:HB3	2.19	0.43
1:B:2279:THR:HG22	1:B:2283:LEU:CG	2.47	0.43
1:A:1040:GLU:O	1:A:1043:LEU:HB2	2.18	0.43
1:A:1313:ARG:CG	1:A:1369:PRO:HG2	2.49	0.43
1:A:1483:MET:CE	1:A:1584:PHE:HB2	2.49	0.43
1:B:2006:LYS:O	1:B:2007:LEU:C	2.57	0.43
1:B:2510:LEU:N	1:B:2510:LEU:HD12	2.34	0.43
1:A:1302:GLN:NE2	1:A:1355:ARG:CA	2.82	0.42
1:A:1357:LEU:HD22	1:A:1397:LEU:CD1	2.49	0.42
1:B:2011:TRP:CZ3	1:B:2247:PRO:CB	3.02	0.42
1:B:2311:LYS:HD3	1:B:2314:MET:HE1	2.01	0.42
1:B:2442:MET:CE	1:B:2535:SER:HB3	2.48	0.42
1:B:2572:ARG:HD3	1:B:2572:ARG:H	1.85	0.42
1:B:2451:ASP:OD1	1:B:2454:LEU:HB2	2.18	0.42
1:B:2499:TYR:HA	1:B:2594:TYR:CZ	2.54	0.42
1:B:2090:ASN:HB3	1:B:2093:LEU:HB2	2.01	0.42
1:B:2174:ARG:HH11	1:B:2498:HIS:HD2	1.66	0.42
1:B:2174:ARG:HG3	1:B:2175:GLY:N	2.34	0.42
1:A:1153:THR:OG1	1:A:1156:ILE:HG13	2.19	0.42
1:A:1061:VAL:HG12	1:A:1065:ASN:HD21	1.84	0.42
1:A:1564:PRO:HB2	1:A:1573:VAL:HG23	2.01	0.42
1:A:1522:MET:HB3	1:A:1599:PRO:HA	2.01	0.42
1:B:2257:TRP:HE3	1:B:2257:TRP:N	2.18	0.42
1:A:1480:ASP:OD2	1:A:1583:ARG:NH1	2.53	0.42
1:B:2011:TRP:CZ3	1:B:2247:PRO:CG	3.03	0.42
1:A:1058:MET:HE1	1:A:1061:VAL:CG2	2.50	0.42
1:A:1110:ILE:HD12	1:A:1270:ASN:HB3	2.02	0.42
1:B:2024:ASN:HD22	1:B:2024:ASN:C	2.23	0.42
1:B:2437:ASN:HD22	1:B:2438:LEU:N	2.17	0.42
1:A:1058:MET:CE	1:A:1061:VAL:HG21	2.50	0.42
1:B:2105:LEU:HD23	2:B:28:HOH:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2218:ARG:O	1:B:2222:GLU:HG3	2.20	0.42
1:A:1095:LYS:O	1:A:1096:ILE:HD12	2.20	0.41
1:B:2313:ARG:CG	1:B:2369:PRO:HG2	2.49	0.41
1:B:2571:PRO:O	1:B:2575:ASP:N	2.51	0.41
1:A:1158:ARG:HG2	1:A:1456:MET:CE	2.49	0.41
1:A:1306:ASP:O	1:A:1310:MET:HB2	2.20	0.41
1:A:1555:ILE:HG22	1:A:1555:ILE:O	2.20	0.41
1:B:2036:TYR:CZ	1:B:2038:GLY:CA	3.03	0.41
1:B:2303:GLU:HA	2:B:196:HOH:O	2.18	0.41
1:A:1310:MET:SD	1:A:1363:MET:HE3	2.61	0.41
1:B:2302:GLN:NE2	1:B:2355:ARG:CA	2.83	0.41
1:A:1196:LYS:HZ1	1:A:1226:GLN:NE2	2.12	0.41
1:A:1257:TRP:N	1:A:1257:TRP:HE3	2.17	0.41
1:A:1372:THR:CG2	1:A:1398:GLN:HB2	2.48	0.41
1:A:1335:THR:OG1	1:A:1370:ASN:ND2	2.52	0.41
1:A:1366:SER:HA	1:A:1367:PRO:HD3	1.86	0.41
1:B:2559:ILE:O	1:B:2559:ILE:HG12	2.20	0.41
1:B:2011:TRP:CD1	1:B:2019:TRP:CH2	3.08	0.41
1:B:2405:MET:O	1:B:2406:ARG:C	2.59	0.41
1:A:1025:VAL:O	1:A:1028:PHE:HB3	2.21	0.41
1:B:2306:ASP:O	1:B:2310:MET:HB2	2.21	0.41
1:B:2406:ARG:HB3	1:B:2407:PRO:HD3	2.03	0.41
1:A:1564:PRO:HB3	1:A:1570:ASP:OD2	2.20	0.41
1:A:1496:ILE:HD11	1:B:2207:LEU:HD21	2.02	0.41
1:A:1598:ILE:HA	1:A:1599:PRO:HD3	1.98	0.41
1:B:2568:ASN:O	1:B:2570:ASP:N	2.54	0.41
1:A:1024:ASN:HD22	1:A:1024:ASN:C	2.23	0.41
1:B:2142:LYS:HE2	1:B:2147:GLY:HA2	2.03	0.41
1:A:1119:GLU:HG2	1:A:1129:LEU:HD12	2.02	0.41
1:A:1157:LEU:HD12	1:A:1157:LEU:HA	1.85	0.41
1:A:1228:ARG:O	1:A:1232:GLN:HG3	2.20	0.41
1:A:1291:LEU:C	1:A:1293:ALA:N	2.74	0.40
1:B:2491:ILE:HD13	1:B:2491:ILE:HA	1.98	0.40
1:A:1449:GLY:O	1:A:1458:VAL:HG22	2.20	0.40
1:A:1499:TYR:HA	1:A:1594:TYR:CZ	2.56	0.40
1:A:1606:ILE:O	1:A:1606:ILE:HG23	2.21	0.40
1:B:2018:ASP:O	1:B:2020:GLN:N	2.54	0.40
1:B:2063:LEU:HD23	1:B:2063:LEU:O	2.21	0.40
1:B:2401:ASN:OD1	1:B:2403:ASP:HB2	2.21	0.40
1:B:2034:THR:HA	1:B:2035:PRO:HD2	1.95	0.40
1:A:1197:LEU:HD22	2:B:184:HOH:O	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1447:ASN:HD21	1:A:1554:ALA:N	2.10	0.40
1:A:1537:SER:OG	1:A:1564:PRO:HG2	2.22	0.40
1:B:2089:ILE:HD12	1:B:2310:MET:CE	2.51	0.40
1:B:2566:PHE:HE2	1:B:2577:ALA:CB	2.34	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	610/624 (98%)	545 (89%)	54 (9%)	11 (2%)	10	32
1	B	610/624 (98%)	539 (88%)	56 (9%)	15 (2%)	6	22
All	All	1220/1248 (98%)	1084 (89%)	110 (9%)	26 (2%)	8	27

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1175	GLY
1	A	1569	ASN
1	B	2175	GLY
1	B	2327	PHE
1	B	2329	GLY
1	A	1173	GLY
1	A	1292	LYS
1	A	1334	ALA
1	A	1370	ASN
1	B	2173	GLY
1	B	2334	ALA
1	B	2370	ASN
1	B	2569	ASN
1	A	1006	LYS

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Mol	Chain	Res	Type
1	B	2091	LYS
1	B	2325	GLU
1	B	2326	LEU
1	A	1327	PHE
1	A	1329	GLY
1	B	2005	GLU
1	B	2019	TRP
1	B	2550	GLU
1	A	1523	ALA
1	A	1046	ALA
1	B	2292	LYS
1	B	2469	VAL

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	502/528 (95%)	470 (94%)	32 (6%)	20	50
1	B	499/528 (94%)	468 (94%)	31 (6%)	21	52
All	All	1001/1056 (95%)	938 (94%)	63 (6%)	21	51

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1004	ASN
1	A	1005	GLU
1	A	1009	THR
1	A	1011	TRP
1	A	1024	ASN
1	A	1032	ASN
1	A	1047	THR
1	A	1063	LEU
1	A	1102	GLU
1	A	1129	LEU
1	A	1132	MET

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Mol	Chain	Res	Type
1	A	1152	TYR
1	A	1157	LEU
1	A	1164	VAL
1	A	1165	LEU
1	A	1182	ARG
1	A	1211	VAL
1	A	1215	GLN
1	A	1219	LEU
1	A	1257	TRP
1	A	1278	ARG
1	A	1308	LEU
1	A	1315	VAL
1	A	1333	TRP
1	A	1343	LEU
1	A	1368	GLU
1	A	1382	ASN
1	A	1437	ASN
1	A	1443	LEU
1	A	1452	GLU
1	A	1473	ASP
1	A	1550	GLU
1	B	2011	TRP
1	B	2024	ASN
1	B	2032	ASN
1	B	2047	THR
1	B	2063	LEU
1	B	2092	GLN
1	B	2102	GLU
1	B	2129	LEU
1	B	2152	TYR
1	B	2164	VAL
1	B	2165	LEU
1	B	2182	ARG
1	B	2211	VAL
1	B	2215	GLN
1	B	2219	LEU
1	B	2257	TRP
1	B	2278	ARG
1	B	2308	LEU
1	B	2315	VAL
1	B	2322	GLU
1	B	2333	TRP

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Mol	Chain	Res	Type
1	B	2343	LEU
1	B	2368	GLU
1	B	2382	ASN
1	B	2437	ASN
1	B	2443	LEU
1	B	2473	ASP
1	B	2559	ILE
1	B	2569	ASN
1	B	2572	ARG
1	B	2609	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1004	ASN
1	A	1024	ASN
1	A	1030	GLN
1	A	1065	ASN
1	A	1090	ASN
1	A	1100	GLN
1	A	1146	GLN
1	A	1204	GLN
1	A	1212	ASN
1	A	1215	GLN
1	A	1226	GLN
1	A	1269	GLN
1	A	1302	GLN
1	A	1428	GLN
1	A	1430	GLN
1	A	1437	ASN
1	A	1447	ASN
1	A	1457	GLN
1	A	1471	ASN
1	A	1498	HIS
1	A	1565	GLN
1	B	2024	ASN
1	B	2030	GLN
1	B	2065	ASN
1	B	2090	ASN
1	B	2100	GLN
1	B	2146	GLN
1	B	2212	ASN

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Mol	Chain	Res	Type
1	B	2215	GLN
1	B	2226	GLN
1	B	2269	GLN
1	B	2302	GLN
1	B	2428	GLN
1	B	2430	GLN
1	B	2437	ASN
1	B	2447	ASN
1	B	2457	GLN
1	B	2471	ASN
1	B	2498	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.