

Full wwPDB X-ray Structure Validation Report (i)

May 17, 2020 - 12:41 am BST

PDB ID	:	1QHM
Title	:	ESCHERICHIA COLI PYRUVATE FORMATE LYASE LARGE DOMAIN
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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 https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity	:	4.02b- 467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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 $(\#Entries)$	${f Similar\ resolution}\ (\#{ m Entries}, { m resolution\ range}({ m \AA}))$	
Clashscore	141614	3569 (2.80-2.80)	
Ramachandran outliers	138981	3498 (2.80-2.80)	
Sidechain outliers	138945	3500 (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 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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of ch	ain	
1	А	624	60%	33%	5% •
1	В	624	58%	35%	5% •



2 Entry composition (i)

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.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	Δ	612	Total	С	Ν	Ο	S	0	0	1
			4794	3034	810	920	30			
1	р	612	Total	С	Ν	Ο	S	0	0	1
	I B		4782	3026	809	917	30	0	0	

• Molecule 1 is a protein called PYRUVATE FORMATE-LYASE.

• Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	125	Total O 125 125	0	0
2	В	109	Total O 109 109	0	0



3 Residue-property plots (i)

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. Residues are colorcoded 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: PYRUVATE FORMATE-LYASE



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4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 65	Depositor
Cell constants	140.80Å 140.80Å 215.90Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 - 2.80	Depositor
% Data completeness	99.0 (20.00-2.80)	Depositor
(in resolution range)	55.0 (20.00 2.00)	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	А	0.46	0/4891	0.66	2/6623~(0.0%)	
1	В	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	$Observed(^{o})$	$Ideal(^{o})$
1	А	1175	GLY	N-CA-C	6.33	128.93	113.10
1	В	2175	GLY	N-CA-C	6.09	128.32	113.10
1	А	1176	ARG	N-CA-C	-5.68	95.66	111.00
1	В	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	А	4794	0	4659	235	0
1	В	4782	0	4636	261	0
2	А	125	0	0	3	0
2	В	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	Clash
Atom-1	Atom-2	distance (Å)	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



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	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



	all pagetti	Interatomic	
Atom-1	Atom-2	distance (\AA)	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	:1465:ILE:HA 1:A:1478:ARG:CZ		0.62
1:A:1465:ILE:HG13	1:A:1478:ARG:CD	1478:ARG:CD 2.21 0.	
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



	A Contraction of the contraction	Interatomic	Clash
Atom-1	Atom-2	$distance (m \AA)$	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	:1158:ARG:HG2 1:A:1456:MET:HE3		0.58
1:A:1207:LEU:HD21	1:B:2496:ILE:HD11	:HD11 1.84 (
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



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	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	A:1420:VAL:HG22 1:A:1430:GLN:OE1 2.08		0.54	
1:A:1004:ASN:HD22	1:A:1005:GLU:N)5:GLU:N 2.06		
1:A:1036:TYR:CZ	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	



		Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	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	



	A L	Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	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	



		Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	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	G2 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	



	• • • • • •	Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	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	:HZ3 1:B:2247:PRO:CG 2.28		0.45	
1:B:2215:GLN:N	LN: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	$2.\overline{46}$	$0.\overline{45}$	
1:A:1095:LYS:H	1:A:1307:HIS:CD2	2.35	0.45	



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Atom-1	Atom-2	distance (Å)	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	0:LEU:N 1:A:1510:LEU:HD12		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	26:GLN:HG3 2.17		
1:A:1311:LYS:HD3	1:A:1314:MET:HE1	IE1 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	



	• • • • •	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	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	



	• • • • • •	Interatomic	Clash	
Atom-1	Atom-2	$distance (m \AA)$	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	1025:VAL:O 1:A:1028:PHE:HB3		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	D2 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	



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 (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	Per	centiles
1	А	610/624~(98%)	545 (89%)	54 (9%)	11 (2%)	8	8 28
1	В	610/624~(98%)	539~(88%)	56 (9%)	15 (2%)	ц.	5 19
All	All	1220/1248~(98%)	1084 (89%)	110 (9%)	26 (2%)	7	7 23

All (26) Ramachandran outliers are listed below:

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



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

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	Perce	ntiles
1	А	502/528~(95%)	470~(94%)	32~(6%)	17	45
1	В	499/528~(94%)	468~(94%)	31~(6%)	18	47
All	All	1001/1056~(95%)	938~(94%)	63~(6%)	18	46

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

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



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



Mol	Chain	Res	Type
1	В	2343	LEU
1	В	2368	GLU
1	В	2382	ASN
1	В	2437	ASN
1	В	2443	LEU
1	В	2473	ASP
1	В	2559	ILE
1	В	2569	ASN
1	В	2572	ARG
1	В	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	А	1004	ASN
1	А	1024	ASN
1	А	1030	GLN
1	А	1065	ASN
1	А	1090	ASN
1	А	1100	GLN
1	А	1146	GLN
1	А	1204	GLN
1	А	1212	ASN
1	А	1215	GLN
1	А	1226	GLN
1	А	1269	GLN
1	А	1302	GLN
1	А	1428	GLN
1	А	1430	GLN
1	А	1437	ASN
1	А	1447	ASN
1	А	1457	GLN
1	А	1471	ASN
1	А	1498	HIS
1	А	1565	GLN
1	В	2024	ASN
1	В	2030	GLN
1	В	2065	ASN
1	В	2090	ASN
1	В	2100	GLN
1	В	2146	GLN
1	В	2212	ASN



		1	1 0
\mathbf{Mol}	Chain	Res	Type
1	В	2215	GLN
1	В	2226	GLN
1	В	2269	GLN
1	В	2302	GLN
1	В	2428	GLN
1	В	2430	GLN
1	В	2437	ASN
1	В	2447	ASN
1	В	2457	GLN
1	В	2471	ASN
1	В	2498	HIS

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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 (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.

