



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:06 AM UTC

PDB ID : 1QHM / pdb_00001qhm
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

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

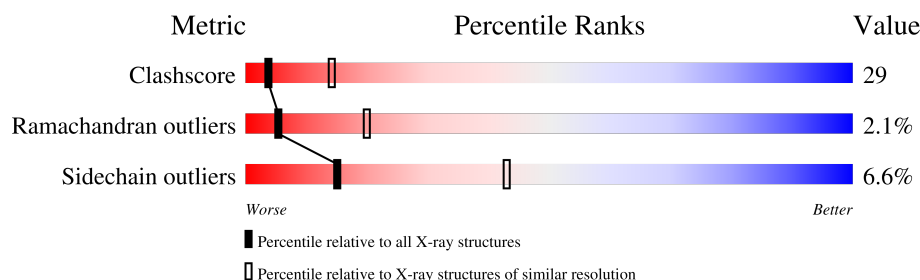
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	624	
1	B	624	

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.

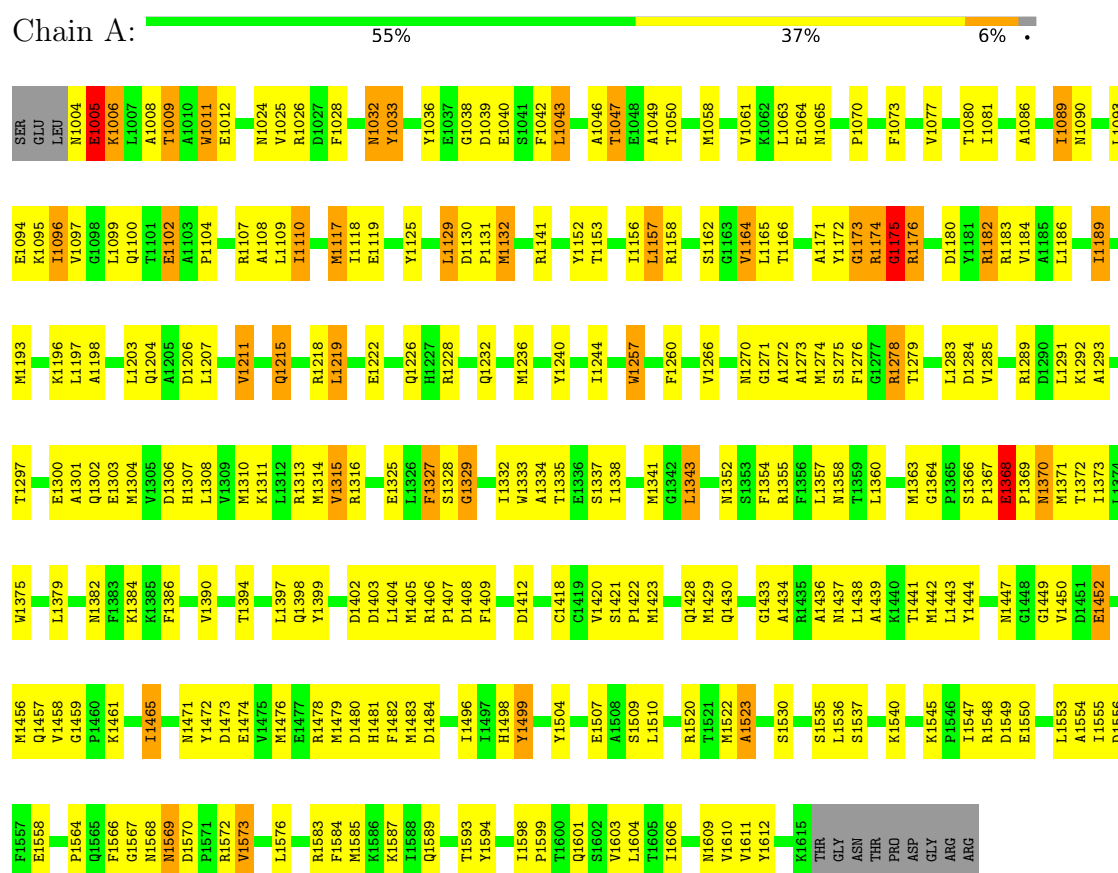
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	125	Total	O	0	0
			125	125		
2	B	109	Total	O	0	0
			109	109		

3 Residue-property plots

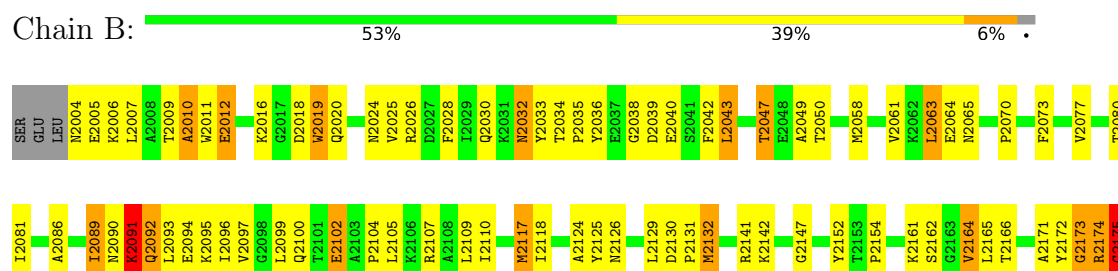
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS was not executed.

• Molecule 1: PYRUVATE FORMATE-LYASE



• Molecule 1: PYRUVATE FORMATE-LYASE





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

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	0.54	0/4891	1.02	28/6623 (0.4%)
1	B	0.54	0/4879	1.05	27/6610 (0.4%)
All	All	0.54	0/9770	1.04	55/13233 (0.4%)

There are no bond length outliers.

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2089	ILE	N-CA-C	-13.61	98.74	111.67
1	A	1089	ILE	N-CA-C	-12.18	100.10	111.67
1	B	2368	GLU	CA-C-N	-10.05	107.28	119.84
1	B	2368	GLU	C-N-CA	-10.05	107.28	119.84
1	A	1368	GLU	CA-C-N	-9.97	107.37	119.84
1	A	1368	GLU	C-N-CA	-9.97	107.37	119.84
1	B	2110	ILE	CA-C-N	9.19	130.13	119.47
1	B	2110	ILE	C-N-CA	9.19	130.13	119.47
1	A	1176	ARG	N-CA-C	-9.14	95.66	109.83
1	B	2176	ARG	N-CA-C	-8.87	96.09	109.83
1	A	1110	ILE	CA-C-N	8.77	129.65	119.47
1	A	1110	ILE	C-N-CA	8.77	129.65	119.47
1	B	2573	VAL	N-CA-C	-7.99	103.97	111.48
1	A	1499	TYR	N-CA-C	-7.80	102.71	111.14
1	B	2433	GLY	N-CA-C	-7.44	101.19	113.02
1	B	2499	TYR	N-CA-C	-7.37	103.18	111.14
1	A	1433	GLY	N-CA-C	-7.36	101.26	112.89
1	A	1272	ALA	N-CA-C	7.32	119.05	111.14
1	A	1332	ILE	N-CA-C	-7.22	99.23	109.63
1	A	1418	CYS	N-CA-C	7.10	120.67	110.10
1	B	2418	CYS	N-CA-C	7.05	120.60	110.10
1	B	2272	ALA	N-CA-C	7.03	118.73	111.14
1	B	2332	ILE	N-CA-C	-6.89	99.71	109.63
1	A	1175	GLY	N-CA-C	6.64	128.93	113.18
1	A	1094	GLU	N-CA-C	6.61	119.81	109.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1573	VAL	N-CA-C	-6.50	106.66	112.12
1	A	1368	GLU	N-CA-C	6.42	121.48	112.75
1	B	2175	GLY	N-CA-C	6.39	128.32	113.18
1	B	2368	GLU	N-CA-C	6.16	121.25	113.25
1	B	2097	VAL	N-CA-C	6.08	117.59	108.96
1	B	2094	GLU	N-CA-C	5.87	118.23	109.25
1	B	2080	THR	N-CA-C	-5.86	101.06	108.45
1	A	1080	THR	N-CA-C	-5.81	101.13	108.45
1	A	1097	VAL	N-CA-C	5.74	117.11	108.96
1	A	1609	ASN	N-CA-C	5.73	119.16	109.76
1	B	2338	ILE	N-CA-C	5.64	117.53	108.85
1	B	2174	ARG	N-CA-C	-5.60	104.66	112.45
1	A	1338	ILE	N-CA-C	5.60	117.47	108.85
1	B	2204	GLN	N-CA-C	5.46	117.23	111.28
1	B	2276	PHE	N-CA-C	-5.42	105.53	111.82
1	B	2077	VAL	N-CA-C	5.34	115.99	108.36
1	A	1189	ILE	N-CA-C	5.32	115.53	110.42
1	B	2012	GLU	CA-C-N	5.30	130.18	122.28
1	B	2012	GLU	C-N-CA	5.30	130.18	122.28
1	B	2447	ASN	N-CA-C	5.28	118.54	112.57
1	A	1174	ARG	N-CA-C	-5.22	105.20	112.45
1	A	1198	ALA	N-CA-C	-5.17	105.33	111.69
1	A	1033	TYR	N-CA-C	-5.16	101.45	109.24
1	A	1077	VAL	N-CA-C	5.16	116.01	108.58
1	B	2189	ILE	N-CA-C	5.16	115.37	110.42
1	A	1548	ARG	N-CA-C	5.15	118.40	110.42
1	A	1276	PHE	N-CA-C	-5.12	105.88	111.82
1	A	1005	GLU	N-CA-C	-5.08	105.20	111.40
1	B	2010	ALA	N-CA-C	5.07	119.46	113.28
1	A	1436	ALA	N-CA-C	-5.05	100.94	109.07

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4794	0	4659	260	0
1	B	4782	0	4636	287	0
2	A	125	0	0	5	0
2	B	109	0	0	5	0
All	All	9810	0	9295	544	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 29.

All (544) 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:H	1:B:2215:GLN:HE21	1.14	0.94
1:A:1465:ILE:HA	1:A:1478:ARG:HH22	1.29	0.93
1:B:2161:LYS:HG2	1:B:2456:MET:HE1	1.52	0.92
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:A:1310:MET:HG2	1:A:1314:MET:HE2	1.57	0.84
1:B:2559:ILE:H	1:B:2559:ILE:HD13	1.40	0.84
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:2058:MET:HE2	1:B:2058:MET:HA	1.63	0.81
1:B:2465:ILE:CG1	1:B:2478:ARG:CZ	2.54	0.81
1:B:2311:LYS:HA	1:B:2314:MET:HE3	1.61	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:2442:MET:HE1	1:B:2535:SER:HB3	1.62	0.80
1:A:1058:MET:HE2	1:A:1058:MET:HA	1.64	0.79
1:B:2032:ASN:N	1:B:2032:ASN:HD22	1.79	0.79
1:A:1311:LYS:HA	1:A:1314:MET:HE3	1.63	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
1:B:2465:ILE:CB	1:B:2478:ARG:NH1	2.49	0.75
1:A:1442:MET:HE1	1:A:1535:SER:HB3	1.68	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:N	1:A:1032:ASN:HD22	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:HE21	1:A:1215:GLN:N	1.88	0.71
1:B:2442:MET:HE1	1:B:2535:SER:CB	2.20	0.71
1:B:2033:TYR:HA	1:B:2285:VAL:HG12	1.72	0.71
1:B:2437:ASN:C	1:B:2437:ASN:HD22	1.99	0.71
1:B:2132:MET:HE3	1:B:2132:MET:HA	1.74	0.70
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:HD13	1:B:2559:ILE:N	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:1437:ASN:C	1:A:1437:ASN:HD22	1.99	0.68
1:A:1196:LYS:NZ	1:A:1226:GLN:HE22	1.91	0.68
1:A:1132:MET:HE3	1:A:1132:MET:HA	1.75	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:OE1	1:A:1368:GLU:HA	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: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:2092:GLN:N	1:B:2092:GLN:CD	2.54	0.65
1:B:2368:GLU:OE1	1:B:2368:GLU:HA	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
1:A:1032:ASN:N	1:A:1032:ASN:ND2	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:1442:MET:HE1	1:A:1535:SER:CB	2.27	0.64
1:A:1423:MET:HE3	1:A:1430:GLN:HB2	1.80	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:2604:LEU:C	1:B:2604:LEU:HD23	2.21	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:2402:ASP:CG	1:B:2406:ARG:NH1	2.57	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:2423:MET:HE3	1:B:2430:GLN:HB2	1.82	0.62
1:A:1402:ASP:CG	1:A:1406:ARG:NH1	2.57	0.62
1:A:1604:LEU:C	1:A:1604:LEU:HD23	2.25	0.62
1:B:2278:ARG:HG2	1:B:2337:SER:HB2	1.81	0.62
1:A:1180:ASP:OD1	1:A:1182:ARG:HD3	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:1458:VAL:HG23	1:A:1459:GLY:N	2.14	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:2464:PRO:C	1:B:2478:ARG:HH12	2.08	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:1476:MET:HE1	1:A:1536:LEU:HD13	1.84	0.60
1:A:1047:THR:HG21	1:A:1303:GLU:OE2	2.02	0.60
1:A:1310:MET:CG	1:A:1363:MET:HE1	2.32	0.60
1:B:2004:ASN:ND2	1:B:2007:LEU:HD13	2.17	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: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:B:2368:GLU:C	1:B:2370:ASN:N	2.61	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:2102:GLU:CD	1:B:2102:GLU:H	2.10	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:1102:GLU:CD	1:A:1102:GLU:H	2.10	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:A:1089:ILE:CD1	1:A:1310:MET:HE3	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1207:LEU:HD21	1:B:2496:ILE:HD11	1.84	0.58
1:B:2310:MET:CG	1:B:2363:MET:HE1	2.33	0.58
1:A:1189:ILE:HG22	1:A:1193:MET:HE2	1.85	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:B:2089:ILE:CD1	1:B:2310:MET:HE3	2.34	0.57
1:A:1291:LEU:C	1:A:1293:ALA:H	2.13	0.57
1:A:1465:ILE:CG1	1:A:1478:ARG:CD	2.81	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:B:2092:GLN:CD	1:B:2092:GLN:H	2.13	0.57
1:B:2189:ILE:HG22	1:B:2193:MET:HE2	1.86	0.57
1:A:1484:ASP:OD1	1:A:1587:LYS:HD2	2.04	0.57
1:B:2476:MET:HE1	1:B:2536:LEU:HD13	1.85	0.57
1:A:1040:GLU:N	1:A:1040:GLU:OE1	2.36	0.57
1:A:1368:GLU:C	1:A:1370:ASN:N	2.61	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
1:B:2470:LEU:HG	1:B:2546:PRO:HG3	1.87	0.56
1:B:2016:LYS:HA	1:B:2020:GLN:CD	2.30	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:2368:GLU:C	1:B:2370:ASN:H	2.13	0.56
1:A:1507:GLU:HB3	1:A:1510:LEU:HD13	1.87	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:A:1368:GLU:C	1:A:1370:ASN:H	2.14	0.55
1:B:2484:ASP:OD1	1:B:2587:LYS:HD2	2.05	0.55
1:B:2310:MET:HG2	1:B:2314:MET:CE	2.32	0.55
1:A:1043:LEU:HD12	1:A:1358:ASN:OD1	2.07	0.55
1:A:1047:THR:CG2	1:A:1049:ALA:H	2.19	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1310:MET:HG2	1:A:1314:MET:CE	2.32	0.55
1:B:2271:GLY:H	1:B:2274:MET:CE	2.19	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:A:1176:ARG:HG3	1:A:1273:ALA:HB3	1.90	0.54
1:B:2117:MET:HE2	1:B:2172:TYR:CD2	2.43	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:1352:ASN:HA	1:A:1355:ARG:HH11	1.73	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: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:2314:MET:HB3	2:B:28:HOH:O	2.06	0.53
1:B:2507:GLU:HB3	1:B:2510:LEU:HD13	1.89	0.53
1:A:1090:ASN:CG	1:A:1093:LEU:HD12	2.32	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:HG22	1:B:2049:ALA:N	2.23	0.53
1:B:2047:THR:CG2	1:B:2049:ALA:H	2.21	0.53
1:A:1421:SER:HB2	1:A:1430:GLN:HE22	1.73	0.53
1:B:2058:MET:HA	1:B:2058:MET:CE	2.37	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:2549:ASP:O	1:B:2550:GLU:C	2.52	0.53
1:B:2570:ASP:O	1:B:2573:VAL:HG22	2.08	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:B:2452:GLU:C	1:B:2454:LEU:H	2.17	0.53
1:B:2040:GLU:OE1	1:B:2040:GLU:N	2.35	0.52
1:B:2310:MET:HG3	1:B:2363:MET:HE1	1.90	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:1117:MET:HE2	1:A:1172:TYR:CD2	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1204:GLN:NE2	1:B:2154:PRO:HD2	2.24	0.52
1:A:1465:ILE:HG13	1:A:1478:ARG:HD2	1.91	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: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: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:1196:LYS:HZ2	1:A:1226:GLN:HE22	1.56	0.50
1:A:1568:ASN:O	1:A:1570:ASP:N	2.43	0.50
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:A:1437:ASN:C	1:A:1437:ASN:ND2	2.68	0.50
1:B:2089:ILE:HD12	1:B:2310:MET:HE3	1.92	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:A:1310:MET:HB2	1:A:1363:MET:HE1	1.94	0.49
1:A:1402:ASP:CG	1:A:1406:ARG:HH12	2.19	0.49
1:B:2109:LEU:HD22	1:B:2118:ILE:CG2	2.41	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2086:ALA:HA	1:B:2240:TYR:CE1	2.47	0.49
1:A:1058:MET:HA	1:A:1058:MET:CE	2.39	0.49
1:A:1437:ASN:HD22	1:A:1439:ALA:H	1.59	0.49
1:A:1456:MET:HE2	1:A:1458:VAL:HG12	1.93	0.49
1:B:2099:LEU:HD11	1:B:2104:PRO:HG3	1.94	0.49
1:B:2402:ASP:CG	1:B:2406:ARG:HH12	2.20	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:A:1310:MET:CB	1:A:1363:MET:HE1	2.42	0.49
1:A:1215:GLN:NE2	1:A:1215:GLN:N	2.55	0.49
1:A:1373:ILE:HD11	1:A:1397:LEU:HD13	1.95	0.49
1:A:1310:MET:HG3	1:A:1363:MET:HE1	1.94	0.49
1:A:1569:ASN:CG	2:A:151:HOH:O	2.55	0.49
1:B:2271:GLY:H	1:B:2274:MET:HE1	1.78	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:B:2604:LEU:HD23	1:B:2604:LEU:O	2.13	0.49
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:1117:MET:HE3	2:A:193:HOH:O	2.14	0.48
1:A:1291:LEU:O	1:A:1293:ALA:N	2.46	0.48
1:B:2291:LEU:C	1:B:2293:ALA:H	2.21	0.48
1:B:2457:GLN:CD	1:B:2461:LYS:HG2	2.38	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:A:1405:MET:O	1:A:1406:ARG:C	2.57	0.48
1:B:2042:PHE:CZ	1:B:2351:LYS:HD2	2.48	0.48
1:A:1117:MET:HE2	1:A:1172:TYR:CE2	2.49	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:A:1028:PHE:CE2	1:A:1285:VAL:HG21	2.48	0.48
1:A:1089:ILE:HD12	1:A:1310:MET:HE3	1.94	0.48
1:A:1403:ASP:OD1	1:A:1406:ARG:NH2	2.46	0.48
1:A:1423:MET:HE2	1:A:1428:GLN:O	2.13	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2006:LYS:O	1:B:2007:LEU:C	2.57	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:B:2089:ILE:HD11	1:B:2314:MET:HE1	1.97	0.47
1:A:1211:VAL:HG22	1:A:1211:VAL:O	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: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:A:1610:VAL:HG23	1:A:1610:VAL:O	2.13	0.47
1:B:2026:ARG:NH2	1:B:2343:LEU:HD23	2.30	0.47
1:B:2073:PHE:HA	1:B:2107:ARG:O	2.13	0.47
1:B:2310:MET:CB	1:B:2363:MET:HE1	2.45	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: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:HG23	1:B:2610:VAL:O	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:2081:ILE:HD11	1:B:2509:SER:HB3	1.97	0.46
1:B:2092:GLN:N	1:B:2092:GLN:OE1	2.48	0.46
1:B:2301:ALA:HA	1:B:2304:MET:HE2	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:B:2437:ASN:C	1:B:2437:ASN:ND2	2.69	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1611:VAL:CG1	1:A:1612:TYR:N	2.78	0.46
1:B:2141:ARG:NH2	1:B:2504:TYR:O	2.48	0.46
1:B:2405:MET:O	1:B:2406:ARG:C	2.59	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:B:2024:ASN:C	1:B:2024:ASN:HD22	2.23	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: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:2117:MET:HE2	1:B:2172:TYR:CE2	2.52	0.45
1:B:2215:GLN:NE2	1:B:2215:GLN:N	2.59	0.45
1:B:2343:LEU:HD22	1:B:2412:ASP:OD2	2.15	0.45
1:B:2403:ASP:HA	1:B:2406:ARG:NH2	2.31	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:B:2423:MET:HE2	1:B:2428:GLN:O	2.16	0.45
1:A:1291:LEU:C	1:A:1293:ALA:N	2.74	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:A:1522:MET:HE2	1:A:1593:THR:HB	1.97	0.45
1:B:2266:VAL:HG12	1:B:2266:VAL:O	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:A:1437:ASN:HD22	1:A:1438:LEU:N	2.13	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:1089:ILE:HD11	1:A:1314:MET:HE1	1.99	0.45
1:A:1095:LYS:H	1:A:1307:HIS:CD2	2.35	0.45
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:1024:ASN:C	1:A:1024:ASN:HD22	2.23	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1420:VAL:HG23	1:A:1523:ALA:HB1	1.98	0.44
1:A:1430:GLN:HG2	1:A:1523:ALA:HB2	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:A:1423:MET:HE2	1:A:1428:GLN:C	2.42	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: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:2172:TYR:O	1:B:2173:GLY:C	2.60	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:1301:ALA:O	1:A:1302:GLN:C	2.61	0.44
1:A:1510:LEU:HD12	1:A:1510:LEU:N	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:1271:GLY:H	1:A:1274:MET:HE1	1.83	0.43
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: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:2310:MET:HB2	1:B:2363:MET:HE1	1.99	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: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
1:B:2130:ASP:OD1	1:B:2130:ASP:C	2.60	0.43
1:B:2324:ASP:C	1:B:2326:LEU:N	2.76	0.43
1:A:1311:LYS:CA	1:A:1314:MET:HE3	2.41	0.43
1:B:2042:PHE:CD1	1:B:2042:PHE:C	2.97	0.43
1:B:2095:LYS:H	1:B:2307:HIS:CD2	2.36	0.43
1:B:2211:VAL:HG22	1:B:2211:VAL:O	2.18	0.43
1:B:2301:ALA:O	1:B:2302:GLN:C	2.61	0.43
1:B:2335:THR:OG1	1:B:2370:ASN:ND2	2.51	0.43
1:B:2420:VAL:HG23	1:B:2523:ALA:HB1	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2459:GLY:HA3	1:B:2482:PHE:HZ	1.84	0.43
1:A:1327:PHE:C	1:A:1329:GLY:N	2.72	0.43
1:B:2403:ASP:OD1	1:B:2406:ARG:NH2	2.47	0.43
1:B:2604:LEU:C	1:B:2604:LEU:CD2	2.92	0.43
1:A:1158:ARG:HG2	1:A:1456:MET:CE	2.49	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:A:1604:LEU:HD23	1:A:1604:LEU:O	2.18	0.43
1:B:2442:MET:HG3	1:B:2479:MET:HE2	2.00	0.43
1:B:2510:LEU:HD12	1:B:2510:LEU:N	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:2572:ARG:HD3	1:B:2572:ARG:H	1.85	0.42
1:A:1130:ASP:OD1	1:A:1130:ASP:C	2.61	0.42
1:A:1423:MET:HE1	2:A:190:HOH:O	2.18	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:2018:ASP:C	1:B:2020:GLN:N	2.77	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:B:2180:ASP:CG	1:B:2182:ARG:HH11	2.27	0.42
1:A:1061:VAL:HG12	1:A:1065:ASN:HD21	1.84	0.42
1:A:1368:GLU:O	1:A:1368:GLU:CD	2.62	0.42
1:A:1522:MET:HB3	1:A:1599:PRO:HA	2.01	0.42
1:A:1564:PRO:HB2	1:A:1573:VAL:HG23	2.01	0.42
1:B:2018:ASP:C	1:B:2020:GLN:H	2.26	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:B:2442:MET:HE1	1:B:2535:SER:HB2	2.00	0.42
1:A:1005:GLU:OE1	1:A:1005:GLU:C	2.62	0.42
1:A:1058:MET:CE	1:A:1061:VAL:HG21	2.50	0.42
1:A:1110:ILE:HD12	1:A:1270:ASN:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2437:ASN:HD22	1:B:2438:LEU:N	2.17	0.42
1:B:2105:LEU:HD23	2:B:28:HOH:O	2.20	0.42
1:B:2124:ALA:C	1:B:2126:ASN:H	2.28	0.42
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:1005:GLU:O	1:A:1006:LYS:C	2.62	0.41
1:A:1306:ASP:O	1:A:1310:MET:HB2	2.20	0.41
1:A:1555:ILE:O	1:A:1555:ILE:HG22	2.20	0.41
1:A:1567:GLY:O	1:A:1568:ASN:C	2.62	0.41
1:B:2036:TYR:CZ	1:B:2038:GLY:CA	3.03	0.41
1:B:2090:ASN:O	1:B:2091:LYS:C	2.62	0.41
1:B:2303:GLU:HA	2:B:196:HOH:O	2.18	0.41
1:A:1089:ILE:HD12	1:A:1310:MET:CE	2.50	0.41
1:A:1172:TYR:O	1:A:1173:GLY:C	2.62	0.41
1:A:1301:ALA:HA	1:A:1304:MET:HE2	2.01	0.41
1:A:1442:MET:HG3	1:A:1479:MET:HE2	2.02	0.41
1:B:2302:GLN:NE2	1:B:2355:ARG:CA	2.83	0.41
1:B:2368:GLU:O	1:B:2368:GLU:CD	2.63	0.41
1:A:1042:PHE:CD1	1:A:1042:PHE:C	2.98	0.41
1:A:1257:TRP:HE3	1:A:1257:TRP:N	2.17	0.41
1:A:1372:THR:CG2	1:A:1398:GLN:HB2	2.48	0.41
1:A:1236:MET:HE3	1:A:1260:PHE:CD1	2.56	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:2423:MET:HE2	1:B:2428:GLN:C	2.46	0.41
1:B:2559:ILE:HG12	1:B:2559:ILE:O	2.20	0.41
1:B:2011:TRP:CD1	1:B:2019:TRP:CH2	3.08	0.41
1:A:1025:VAL:O	1:A:1028:PHE:HB3	2.21	0.41
1:B:2271:GLY:H	1:B:2274:MET:HE3	1.85	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:B:2522:MET:HE2	1:B:2593:THR:HB	2.02	0.41
1:A:1183:ARG:O	1:A:1184:VAL:C	2.64	0.41
1:A:1496:ILE:HD11	1:B:2207:LEU:HD21	2.02	0.41
1:A:1564:PRO:HB3	1:A:1570:ASP:OD2	2.20	0.41
1:B:2236:MET:HE3	1:B:2260:PHE:CD1	2.56	0.41
1:B:2279:THR:O	1:B:2280:SER:C	2.63	0.41
1:A:1180:ASP:CG	1:A:1182:ARG:HH11	2.29	0.41
1:A:1327:PHE:O	1:A:1328:SER:C	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1598:ILE:HA	1:A:1599:PRO:HD3	1.98	0.41
1:B:2142:LYS:HE2	1:B:2147:GLY:HA2	2.03	0.41
1:B:2452:GLU:C	1:B:2452:GLU:CD	2.89	0.41
1:B:2452:GLU:CD	1:B:2453:LYS:N	2.79	0.41
1:B:2568:ASN:O	1:B:2570:ASP:N	2.54	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: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:O	1:B:2063:LEU:HD23	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:B:2573:VAL:C	1:B:2575:ASP:N	2.77	0.40
1:A:1197:LEU:HD22	2:B:184:HOH:O	2.20	0.40
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	Percentiles	
1	A	610/624 (98%)	545 (89%)	54 (9%)	11 (2%)	6	23
1	B	610/624 (98%)	539 (88%)	56 (9%)	15 (2%)	4	16
All	All	1220/1248 (98%)	1084 (89%)	110 (9%)	26 (2%)	5	20

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
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%)	468 (93%)	34 (7%)	14	42
1	B	499/528 (94%)	467 (94%)	32 (6%)	16	44
All	All	1001/1056 (95%)	935 (93%)	66 (7%)	15	43

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1005	GLU
1	A	1009	THR
1	A	1011	TRP
1	A	1032	ASN
1	A	1043	LEU
1	A	1047	THR
1	A	1063	LEU
1	A	1096	ILE
1	A	1102	GLU
1	A	1117	MET
1	A	1129	LEU
1	A	1132	MET
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	1289	ARG
1	A	1308	LEU
1	A	1315	VAL
1	A	1343	LEU
1	A	1368	GLU
1	A	1382	ASN
1	A	1443	LEU
1	A	1452	GLU
1	A	1465	ILE
1	A	1473	ASP
1	A	1545	LYS
1	A	1550	GLU
1	B	2032	ASN
1	B	2043	LEU
1	B	2047	THR
1	B	2063	LEU
1	B	2091	LYS
1	B	2092	GLN
1	B	2096	ILE
1	B	2102	GLU

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Mol	Chain	Res	Type
1	B	2117	MET
1	B	2129	LEU
1	B	2132	MET
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	2289	ARG
1	B	2308	LEU
1	B	2315	VAL
1	B	2322	GLU
1	B	2343	LEU
1	B	2368	GLU
1	B	2382	ASN
1	B	2443	LEU
1	B	2473	ASP
1	B	2559	ILE
1	B	2572	ARG
1	B	2609	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) 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	1126	ASN
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

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Mol	Chain	Res	Type
1	A	1430	GLN
1	A	1437	ASN
1	A	1447	ASN
1	A	1457	GLN
1	A	1471	ASN
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	2126	ASN
1	B	2204	GLN
1	B	2212	ASN
1	B	2215	GLN
1	B	2226	GLN
1	B	2269	GLN
1	B	2302	GLN
1	B	2430	GLN
1	B	2437	ASN
1	B	2447	ASN
1	B	2457	GLN
1	B	2471	ASN
1	B	2609	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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.