



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:35 AM UTC

PDB ID : 1ZJH / pdb_00001zjh
Title : Structure of human muscle pyruvate kinase (PKM2)
Authors : Choe, J.; Atanassova, A.; Arrowsmith, C.; Edwards, A.; Sundstrom, M.;
Bochkarev, A.; Park, H.; Structural Genomics Consortium (SGC)
Deposited on : 2005-04-28
Resolution : 2.20 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)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

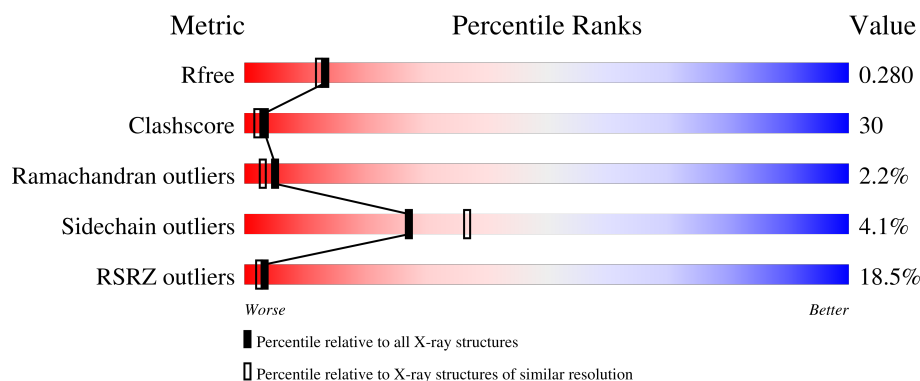
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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))
R_{free}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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 $\leq 5\%$. 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.

Mol	Chain	Length	Quality of chain
1	A	548	17% 55% 33% 5% 7%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4004 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 kinase, isozymes M1/M2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	507	Total	C	N	O	S	0	0	0
			3882	2443	688	727	24			

There are 19 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-17	MET	-	cloning artifact	UNP P14618
A	-16	GLY	-	cloning artifact	UNP P14618
A	-15	SER	-	cloning artifact	UNP P14618
A	-14	SER	-	cloning artifact	UNP P14618
A	-13	HIS	-	expression tag	UNP P14618
A	-12	HIS	-	expression tag	UNP P14618
A	-11	HIS	-	expression tag	UNP P14618
A	-10	HIS	-	expression tag	UNP P14618
A	-9	HIS	-	expression tag	UNP P14618
A	-8	HIS	-	expression tag	UNP P14618
A	-7	SER	-	cloning artifact	UNP P14618
A	-6	SER	-	cloning artifact	UNP P14618
A	-5	GLY	-	cloning artifact	UNP P14618
A	-4	LEU	-	cloning artifact	UNP P14618
A	-3	VAL	-	cloning artifact	UNP P14618
A	-2	PRO	-	cloning artifact	UNP P14618
A	-1	ARG	-	cloning artifact	UNP P14618
A	0	GLY	-	cloning artifact	UNP P14618
A	1	SER	-	cloning artifact	UNP P14618

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	122	Total	O	0	0
			122	122		

4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	86.45Å 111.29Å 126.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.11 – 2.20 29.11 – 2.20	Depositor EDS
% Data completeness (in resolution range)	96.9 (29.11-2.20) 96.8 (29.11-2.20)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.60 (at 2.20Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.231 , 0.279 0.230 , 0.280	Depositor DCC
R_{free} test set	1553 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	34.2	Xtriage
Anisotropy	0.084	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 42.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4004	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.64% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	0.48	0/3945	0.88	5/5327 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	287	ASP	N-CA-C	-6.66	105.31	113.50
1	A	114	LYS	N-CA-C	-6.50	104.28	111.36
1	A	405	SER	N-CA-C	-5.35	105.58	113.61
1	A	334	ILE	N-CA-C	-5.30	105.96	111.58
1	A	299	GLU	N-CA-C	5.18	116.92	111.28

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	3882	0	3972	238	0
2	A	122	0	0	3	0
All	All	4004	0	3972	238	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 30.

All (238) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:THR:HG22	1:A:72:ARG:HD3	1.30	1.11
1:A:326:ALA:HB2	1:A:359:MET:HB3	1.45	0.98
1:A:122:LEU:HD12	1:A:149:GLU:HG2	1.56	0.87
1:A:358:ILE:HD12	1:A:358:ILE:O	1.75	0.87
1:A:46:ILE:HD12	1:A:358:ILE:HD11	1.55	0.86
1:A:49:THR:CG2	1:A:72:ARG:HH11	1.92	0.81
1:A:131:VAL:HG12	1:A:153:GLU:HB3	1.62	0.81
1:A:47:ILE:HD13	1:A:357:CYS:HB3	1.63	0.80
1:A:49:THR:HG21	1:A:72:ARG:HH11	1.47	0.79
1:A:270:ILE:CD1	1:A:289:ILE:HG23	2.13	0.78
1:A:270:ILE:HD13	1:A:289:ILE:HG23	1.65	0.77
1:A:118:ILE:HD13	2:A:686:HOH:O	1.83	0.77
1:A:441:ALA:HB2	1:A:468:ILE:HD11	1.68	0.76
1:A:427:ILE:HB	1:A:449:ILE:HD13	1.67	0.75
1:A:326:ALA:HB1	1:A:359:MET:HE2	1.68	0.75
1:A:441:ALA:CB	1:A:468:ILE:HD11	2.16	0.75
1:A:261:GLY:HA2	1:A:264:ILE:HD13	1.68	0.74
1:A:428:ILE:HD11	1:A:493:MET:HE3	1.70	0.74
1:A:47:ILE:CD1	1:A:357:CYS:HB3	2.18	0.74
1:A:132:GLU:HB3	1:A:201:SER:HA	1.69	0.73
1:A:141:ILE:CD1	1:A:156:LEU:HD23	2.18	0.73
1:A:49:THR:HG22	1:A:72:ARG:CD	2.17	0.72
1:A:46:ILE:HD12	1:A:358:ILE:CD1	2.20	0.71
1:A:468:ILE:HD12	1:A:468:ILE:N	2.05	0.70
1:A:270:ILE:N	1:A:270:ILE:HD12	2.08	0.69
1:A:261:GLY:CA	1:A:264:ILE:HD13	2.23	0.69
1:A:174:TYR:HB3	1:A:178:GLY:HA2	1.73	0.69
1:A:87:ILE:HD12	1:A:109:VAL:HG11	1.74	0.69
1:A:122:LEU:HD23	1:A:204:SER:HB3	1.75	0.69
1:A:188:GLY:HA3	1:A:191:PHE:CE2	2.28	0.67
1:A:24:THR:HG22	1:A:27:GLU:H	1.60	0.66
1:A:118:ILE:N	1:A:118:ILE:HD12	2.11	0.66
1:A:326:ALA:CB	1:A:359:MET:HE2	2.25	0.66
1:A:45:GLY:C	1:A:46:ILE:HD13	2.20	0.66
1:A:465:TYR:O	1:A:468:ILE:HD13	1.97	0.65
1:A:326:ALA:CB	1:A:359:MET:HB3	2.23	0.65
1:A:42:ARG:HE	1:A:378:HIS:HD2	1.45	0.65
1:A:49:THR:HG23	1:A:360:LEU:O	1.96	0.65
1:A:254:ARG:CZ	1:A:266:ILE:HD12	2.27	0.65
1:A:403:ILE:H	1:A:403:ILE:HD12	1.62	0.65
1:A:42:ARG:HE	1:A:378:HIS:CD2	2.14	0.64
1:A:360:LEU:HD21	1:A:377:GLN:OE1	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:ILE:HD13	1:A:377:GLN:CG	2.28	0.63
1:A:430:LEU:HD22	1:A:512:THR:HG22	1.80	0.63
1:A:196:VAL:HG12	1:A:198:ASN:O	1.98	0.63
1:A:219:ALA:HB3	1:A:252:GLU:HG2	1.80	0.63
1:A:47:ILE:N	1:A:47:ILE:HD12	2.14	0.63
1:A:381:ALA:O	1:A:385:GLU:HG3	1.99	0.63
1:A:34:ILE:HD13	1:A:34:ILE:H	1.65	0.62
1:A:141:ILE:HD13	1:A:156:LEU:HB3	1.81	0.62
1:A:261:GLY:C	1:A:264:ILE:HD13	2.24	0.62
1:A:182:LEU:HD23	1:A:196:VAL:HA	1.82	0.61
1:A:270:ILE:HD11	1:A:289:ILE:HD12	1.83	0.61
1:A:87:ILE:HD12	1:A:109:VAL:CG1	2.29	0.61
1:A:144:ASP:OD2	1:A:146:ALA:HB3	2.01	0.61
1:A:445:PRO:HG3	1:A:449:ILE:HD11	1.81	0.61
1:A:46:ILE:C	1:A:47:ILE:HD12	2.25	0.61
1:A:123:ILE:HG23	1:A:151:CYS:O	2.01	0.61
1:A:428:ILE:CD1	1:A:493:MET:HE3	2.30	0.61
1:A:427:ILE:HB	1:A:449:ILE:CD1	2.31	0.60
1:A:493:MET:HE2	1:A:493:MET:HA	1.83	0.60
1:A:439:GLN:O	1:A:442:ARG:HG2	2.01	0.60
1:A:58:GLU:CD	1:A:58:GLU:H	2.08	0.60
1:A:225:ILE:O	1:A:229:LYS:HG2	2.02	0.60
1:A:404:THR:HG21	1:A:409:GLU:HB3	1.84	0.59
1:A:198:ASN:CG	1:A:199:GLY:H	2.10	0.59
1:A:313:ILE:HD13	1:A:323:VAL:CG2	2.32	0.59
1:A:56:SER:HB2	1:A:58:GLU:OE1	2.03	0.59
1:A:427:ILE:CD1	1:A:447:ALA:HB3	2.33	0.59
1:A:31:ARG:HG3	1:A:31:ARG:HH11	1.68	0.59
1:A:330:LEU:O	1:A:363:GLU:HG2	2.02	0.59
1:A:264:ILE:N	1:A:264:ILE:HD12	2.19	0.58
1:A:395:GLU:OE1	1:A:398:ARG:HD3	2.02	0.58
1:A:105:ARG:NH2	1:A:470:PRO:O	2.37	0.58
1:A:338:ARG:HG3	1:A:338:ARG:HH11	1.68	0.58
1:A:313:ILE:HD13	1:A:323:VAL:CG1	2.34	0.57
1:A:515:ARG:HG3	1:A:515:ARG:HH11	1.70	0.57
1:A:123:ILE:HD13	1:A:204:SER:HA	1.86	0.57
1:A:46:ILE:HD12	1:A:358:ILE:CG1	2.34	0.57
1:A:49:THR:HG22	1:A:72:ARG:HH11	1.68	0.56
1:A:338:ARG:HH22	1:A:341:ARG:CZ	2.19	0.56
1:A:123:ILE:HD12	1:A:123:ILE:N	2.20	0.56
1:A:270:ILE:CD1	1:A:270:ILE:N	2.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:VAL:CG1	1:A:153:GLU:HB3	2.36	0.56
1:A:141:ILE:HD11	1:A:156:LEU:HD23	1.87	0.55
1:A:120:THR:O	1:A:205:LYS:HA	2.06	0.55
1:A:123:ILE:HA	1:A:151:CYS:HB2	1.89	0.55
1:A:389:TYR:HE1	1:A:391:LEU:HB3	1.69	0.55
1:A:347:VAL:O	1:A:351:VAL:HG12	2.06	0.55
1:A:47:ILE:HG13	1:A:70:VAL:HB	1.88	0.55
1:A:358:ILE:HD12	1:A:358:ILE:C	2.30	0.55
1:A:496:GLY:HA3	1:A:502:PHE:CZ	2.42	0.55
1:A:366:LYS:O	1:A:367:GLY:O	2.25	0.55
1:A:132:GLU:CB	1:A:201:SER:HA	2.37	0.54
1:A:167:VAL:HG13	1:A:171:SER:HB2	1.88	0.54
1:A:169:VAL:HA	1:A:184:VAL:HG12	1.89	0.54
1:A:270:ILE:HD11	1:A:289:ILE:HG23	1.88	0.54
1:A:167:VAL:CG1	1:A:184:VAL:HG21	2.36	0.54
1:A:186:GLN:HE21	1:A:193:VAL:HG21	1.72	0.54
1:A:465:TYR:CB	1:A:468:ILE:HD13	2.38	0.54
1:A:465:TYR:C	1:A:468:ILE:HD13	2.33	0.54
1:A:49:THR:HG21	1:A:72:ARG:NH1	2.18	0.53
1:A:246:LYS:HG2	1:A:249:ASP:OD2	2.09	0.53
1:A:487:LEU:C	1:A:487:LEU:HD23	2.34	0.53
1:A:134:LYS:HD2	1:A:134:LYS:N	2.23	0.53
1:A:152:ASP:CG	1:A:153:GLU:N	2.67	0.53
1:A:335:LYS:C	1:A:369:TYR:HE2	2.16	0.53
1:A:348:ALA:O	1:A:351:VAL:HG13	2.08	0.53
1:A:407:PRO:HB2	1:A:520:PHE:CE2	2.44	0.53
1:A:34:ILE:H	1:A:34:ILE:CD1	2.22	0.53
1:A:358:ILE:CD1	1:A:377:GLN:CG	2.86	0.53
1:A:260:LYS:NZ	1:A:260:LYS:HB3	2.24	0.52
1:A:120:THR:HG22	1:A:158:LEU:CD2	2.39	0.52
1:A:167:VAL:HG13	1:A:171:SER:CB	2.39	0.52
1:A:117:GLU:OE2	1:A:119:ARG:HD3	2.10	0.52
1:A:140:LYS:HG2	1:A:193:VAL:HG12	1.91	0.52
1:A:271:GLU:O	1:A:299:GLU:HG3	2.10	0.52
1:A:331:GLU:O	1:A:334:ILE:HG12	2.09	0.52
1:A:261:GLY:HA2	1:A:264:ILE:CD1	2.39	0.52
1:A:324:ILE:HD12	1:A:324:ILE:N	2.24	0.52
1:A:330:LEU:C	1:A:363:GLU:HG2	2.34	0.52
1:A:168:GLU:HA	1:A:187:LYS:HD2	1.90	0.51
1:A:123:ILE:N	1:A:123:ILE:CD1	2.74	0.51
1:A:454:ARG:HG2	1:A:454:ARG:HH11	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:ASN:O	1:A:148:MET:HG3	2.11	0.51
1:A:361:SER:N	1:A:363:GLU:OE2	2.44	0.51
1:A:167:VAL:HG11	1:A:184:VAL:HG21	1.92	0.51
1:A:186:GLN:HB2	1:A:193:VAL:CG2	2.41	0.51
1:A:468:ILE:N	1:A:468:ILE:CD1	2.72	0.51
1:A:134:LYS:HD2	1:A:134:LYS:H	1.76	0.50
1:A:317:ASN:HD21	1:A:354:GLY:HA3	1.76	0.50
1:A:117:GLU:C	1:A:118:ILE:HD12	2.36	0.50
1:A:334:ILE:HG23	1:A:367:GLY:HA2	1.93	0.50
1:A:493:MET:HE1	1:A:508:VAL:HG21	1.94	0.50
1:A:287:ASP:O	1:A:322:PRO:HD2	2.10	0.50
1:A:47:ILE:HD11	1:A:357:CYS:SG	2.52	0.50
1:A:51:GLY:O	1:A:55:ARG:HB2	2.12	0.50
1:A:180:ILE:N	1:A:180:ILE:HD12	2.26	0.50
1:A:198:ASN:ND2	1:A:199:GLY:N	2.59	0.50
1:A:335:LYS:HG3	1:A:336:LYS:HD2	1.94	0.50
1:A:372:GLU:CD	1:A:372:GLU:H	2.20	0.50
1:A:446:ARG:CG	2:A:660:HOH:O	2.60	0.50
1:A:419:SER:OG	1:A:427:ILE:HD11	2.11	0.50
1:A:358:ILE:CD1	1:A:377:GLN:HG3	2.42	0.50
1:A:446:ARG:HG2	2:A:660:HOH:O	2.11	0.50
1:A:335:LYS:C	1:A:336:LYS:HD2	2.37	0.49
1:A:471:VAL:HG11	1:A:495:VAL:HG11	1.94	0.49
1:A:132:GLU:HB2	1:A:200:GLY:O	2.12	0.49
1:A:519:GLY:O	1:A:520:PHE:HB2	2.12	0.49
1:A:118:ILE:N	1:A:118:ILE:CD1	2.76	0.49
1:A:158:LEU:HD22	1:A:208:VAL:HG21	1.95	0.49
1:A:122:LEU:HB2	1:A:149:GLU:HA	1.95	0.49
1:A:123:ILE:HG21	1:A:131:VAL:HG23	1.93	0.49
1:A:264:ILE:N	1:A:264:ILE:CD1	2.76	0.48
1:A:123:ILE:CD1	1:A:203:GLY:O	2.61	0.48
1:A:403:ILE:HD12	1:A:403:ILE:N	2.27	0.48
1:A:179:LEU:HB2	1:A:180:ILE:HD12	1.95	0.48
1:A:481:TRP:CB	1:A:516:PRO:HB3	2.43	0.48
1:A:452:VAL:HG21	1:A:492:ALA:HB2	1.96	0.48
1:A:198:ASN:ND2	1:A:199:GLY:H	2.12	0.48
1:A:313:ILE:HD13	1:A:323:VAL:HG21	1.96	0.48
1:A:47:ILE:CD1	1:A:47:ILE:N	2.75	0.48
1:A:356:ASP:HA	1:A:466:ARG:HB2	1.95	0.48
1:A:515:ARG:HB3	1:A:516:PRO:HD2	1.96	0.47
1:A:430:LEU:HD22	1:A:512:THR:CG2	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:ILE:CG2	1:A:164:CYS:N	2.78	0.46
1:A:493:MET:HE2	1:A:502:PHE:CZ	2.50	0.46
1:A:338:ARG:HH12	1:A:341:ARG:NH1	2.14	0.46
1:A:441:ALA:HB1	1:A:468:ILE:HD11	1.96	0.46
1:A:55:ARG:NH2	1:A:85:GLU:HB3	2.31	0.46
1:A:495:VAL:O	1:A:499:ARG:HG2	2.16	0.46
1:A:27:GLU:O	1:A:31:ARG:HG2	2.16	0.46
1:A:186:GLN:HB2	1:A:193:VAL:HG21	1.97	0.46
1:A:73:LEU:HD22	1:A:87:ILE:HD11	1.98	0.45
1:A:465:TYR:HB2	1:A:468:ILE:HD13	1.98	0.45
1:A:333:MET:HE3	1:A:337:PRO:O	2.17	0.45
1:A:34:ILE:HD13	1:A:34:ILE:N	2.29	0.45
1:A:47:ILE:HD11	1:A:357:CYS:HB3	1.99	0.45
1:A:313:ILE:HD13	1:A:323:VAL:HG11	1.99	0.44
1:A:493:MET:CE	1:A:508:VAL:HG21	2.48	0.44
1:A:340:THR:OG1	1:A:343:GLU:HG3	2.18	0.44
1:A:397:LEU:HD13	1:A:442:ARG:O	2.18	0.44
1:A:132:GLU:HB2	1:A:200:GLY:C	2.42	0.44
1:A:87:ILE:CD1	1:A:109:VAL:CG1	2.95	0.44
1:A:167:VAL:HG12	1:A:168:GLU:N	2.33	0.44
1:A:446:ARG:HG3	1:A:447:ALA:N	2.33	0.43
1:A:152:ASP:CG	1:A:153:GLU:H	2.27	0.43
1:A:147:TYR:CD1	1:A:155:ILE:HD13	2.53	0.43
1:A:198:ASN:CG	1:A:199:GLY:N	2.76	0.43
1:A:415:ALA:HB2	1:A:511:LEU:HD21	2.00	0.43
1:A:45:GLY:O	1:A:46:ILE:HD13	2.17	0.43
1:A:135:LYS:C	1:A:137:ALA:H	2.27	0.43
1:A:329:MET:HG3	1:A:359:MET:O	2.18	0.43
1:A:385:GLU:HA	1:A:388:ILE:HD12	2.01	0.43
1:A:58:GLU:CD	1:A:58:GLU:N	2.75	0.43
1:A:481:TRP:CG	1:A:516:PRO:HB3	2.54	0.43
1:A:105:ARG:NE	1:A:105:ARG:HA	2.34	0.42
1:A:270:ILE:HD13	1:A:289:ILE:CG2	2.44	0.42
1:A:31:ARG:HG3	1:A:31:ARG:NH1	2.33	0.42
1:A:46:ILE:HD12	1:A:358:ILE:HG13	2.01	0.42
1:A:267:ILE:HG21	1:A:324:ILE:HD13	2.00	0.42
1:A:394:PHE:HE1	1:A:417:GLU:OE2	2.03	0.42
1:A:111:LEU:HD23	1:A:111:LEU:C	2.45	0.42
1:A:427:ILE:HD12	1:A:447:ALA:HB3	2.01	0.42
1:A:123:ILE:HA	1:A:151:CYS:O	2.20	0.42
1:A:475:ASP:HB2	1:A:487:LEU:HD21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:ILE:HD11	1:A:203:GLY:O	2.20	0.42
1:A:454:ARG:NH1	1:A:475:ASP:O	2.50	0.42
1:A:454:ARG:HG2	1:A:454:ARG:NH1	2.34	0.42
1:A:245:ARG:C	1:A:282:ILE:HD11	2.45	0.42
1:A:87:ILE:CD1	1:A:109:VAL:HG11	2.45	0.41
1:A:181:SER:H	1:A:198:ASN:HB3	1.84	0.41
1:A:338:ARG:HG3	1:A:338:ARG:NH1	2.32	0.41
1:A:454:ARG:O	1:A:456:PRO:HD3	2.21	0.41
1:A:25:PHE:O	1:A:28:HIS:HB3	2.21	0.41
1:A:120:THR:HG22	1:A:158:LEU:HD21	2.01	0.41
1:A:205:LYS:O	1:A:205:LYS:HG3	2.20	0.41
1:A:245:ARG:HB2	1:A:274:GLU:HG2	2.02	0.41
1:A:422:CYS:O	1:A:423:CYS:C	2.62	0.41
1:A:167:VAL:CG1	1:A:168:GLU:N	2.84	0.41
1:A:152:ASP:C	1:A:154:ASN:H	2.28	0.41
1:A:169:VAL:HA	1:A:184:VAL:CG1	2.49	0.41
1:A:193:VAL:O	1:A:193:VAL:HG23	2.20	0.41
1:A:230:PHE:O	1:A:233:GLU:HG2	2.20	0.41
1:A:25:PHE:HE1	1:A:29:MET:SD	2.44	0.41
1:A:55:ARG:NH2	1:A:85:GLU:OE1	2.51	0.41
1:A:163:ILE:HG23	1:A:164:CYS:N	2.36	0.41
1:A:416:VAL:HG21	1:A:443:TYR:HB2	2.01	0.41
1:A:130:GLU:HG2	1:A:203:GLY:HA2	2.03	0.41
1:A:452:VAL:CG2	1:A:492:ALA:HB2	2.50	0.41
1:A:336:LYS:HD2	1:A:336:LYS:N	2.35	0.40
1:A:409:GLU:O	1:A:413:VAL:HG23	2.20	0.40
1:A:147:TYR:CD2	1:A:155:ILE:HD11	2.56	0.40
1:A:222:GLU:HA	1:A:225:ILE:HD12	2.03	0.40
1:A:330:LEU:HG	1:A:339:PRO:HB3	2.03	0.40
1:A:376:MET:O	1:A:380:ILE:HG12	2.22	0.40
1:A:426:ALA:HA	1:A:447:ALA:HB1	2.04	0.40
1:A:115:GLY:HA2	1:A:224:ASP:OD2	2.22	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	505/548 (92%)	471 (93%)	23 (5%)	11 (2%)	5 3

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	516	PRO
1	A	367	GLY
1	A	519	GLY
1	A	520	PHE
1	A	124	LYS
1	A	327	THR
1	A	326	ALA
1	A	517	GLY
1	A	148	MET
1	A	333	MET
1	A	475	ASP

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	418/450 (93%)	401 (96%)	17 (4%)	27 37

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	ILE
1	A	46	ILE
1	A	47	ILE
1	A	96	SER
1	A	105	ARG
1	A	118	ILE

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Mol	Chain	Res	Type
1	A	123	ILE
1	A	132	GLU
1	A	163	ILE
1	A	186	GLN
1	A	260	LYS
1	A	264	ILE
1	A	270	ILE
1	A	284	GLU
1	A	351	VAL
1	A	468	ILE
1	A	527	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	ASN
1	A	77	HIS
1	A	154	ASN
1	A	183	GLN
1	A	186	GLN
1	A	198	ASN
1	A	209	ASN
1	A	317	ASN
1	A	377	GLN
1	A	378	HIS
1	A	490	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

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 ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	507/548 (92%)	0.77	94 (18%) 3 2	22, 36, 74, 95	0

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	327	THR	7.4
1	A	514	TRP	6.7
1	A	133	LEU	5.8
1	A	520	PHE	5.1
1	A	330	LEU	4.6
1	A	334	ILE	4.6
1	A	516	PRO	4.6
1	A	123	ILE	4.5
1	A	335	LYS	4.2
1	A	389	TYR	3.7
1	A	137	ALA	3.6
1	A	131	VAL	3.6
1	A	326	ALA	3.5
1	A	521	THR	3.4
1	A	39	ILE	3.4
1	A	152	ASP	3.4
1	A	517	GLY	3.3
1	A	194	THR	3.3
1	A	399	ARG	3.3
1	A	140	LYS	3.2
1	A	155	ILE	3.2
1	A	328	GLN	3.2
1	A	134	LYS	3.2
1	A	370	PRO	3.1
1	A	124	LYS	3.1
1	A	481	TRP	3.0
1	A	139	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	477	VAL	3.0
1	A	127	GLY	3.0
1	A	138	THR	2.9
1	A	126	SER	2.9
1	A	188	GLY	2.9
1	A	148	MET	2.8
1	A	329	MET	2.8
1	A	173	ILE	2.7
1	A	166	VAL	2.7
1	A	513	GLY	2.7
1	A	179	LEU	2.7
1	A	193	VAL	2.7
1	A	180	ILE	2.7
1	A	398	ARG	2.7
1	A	518	SER	2.6
1	A	143	LEU	2.6
1	A	202	LEU	2.5
1	A	24	THR	2.5
1	A	298	ILE	2.5
1	A	189	ALA	2.5
1	A	203	GLY	2.5
1	A	362	GLY	2.5
1	A	132	GLU	2.5
1	A	331	GLU	2.5
1	A	125	GLY	2.4
1	A	163	ILE	2.4
1	A	191	PHE	2.4
1	A	391	LEU	2.4
1	A	397	LEU	2.4
1	A	170	GLY	2.3
1	A	34	ILE	2.3
1	A	196	VAL	2.3
1	A	372	GLU	2.3
1	A	135	LYS	2.3
1	A	192	LEU	2.3
1	A	37	PRO	2.3
1	A	339	PRO	2.3
1	A	38	PRO	2.3
1	A	129	ALA	2.3
1	A	141	ILE	2.3
1	A	167	VAL	2.3
1	A	184	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	128	THR	2.2
1	A	403	ILE	2.2
1	A	158	LEU	2.2
1	A	151	CYS	2.2
1	A	480	ALA	2.2
1	A	147	TYR	2.2
1	A	400	LEU	2.2
1	A	338	ARG	2.1
1	A	393	LEU	2.1
1	A	58	GLU	2.1
1	A	169	VAL	2.1
1	A	32	LEU	2.1
1	A	395	GLU	2.1
1	A	118	ILE	2.1
1	A	369	TYR	2.1
1	A	130	GLU	2.1
1	A	197	GLU	2.1
1	A	156	LEU	2.1
1	A	390	HIS	2.1
1	A	153	GLU	2.0
1	A	392	GLN	2.0
1	A	512	THR	2.0
1	A	146	ALA	2.0
1	A	177	ASP	2.0
1	A	150	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.