WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Oct 23, 2021 – 11:14 AM EDT

PDB ID	:	1AUP
Title	:	GLUTAMATE DEHYDROGENASE
Authors	:	Baker, P.J.; Waugh, M.L.; Stillman, T.J.; Turnbull, A.P.; Rice, D.W.
Deposited on	:	1997-09-01
Resolution	:	2.50 Å(reported)

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

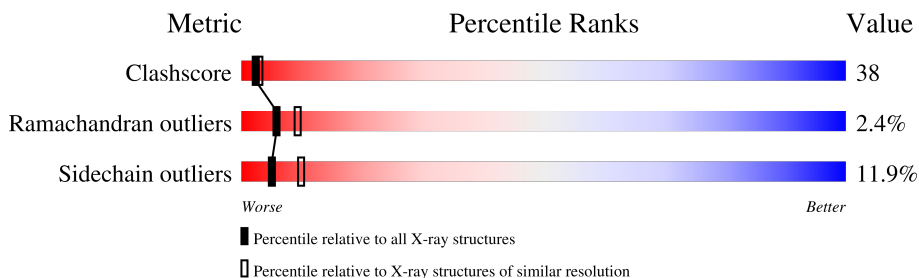|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 2.50 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	Percentile Ranks	Value
Clashscore		38
Ramachandran outliers		2.4%
Sidechain outliers		11.9%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	449	48% 38% 8% 5%

2 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 3315 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 NAD-SPECIFIC GLUTAMATE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	427	Total 3275	C 2083	N 547	O 627	S 18	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	89	LEU	LYS	engineered mutation	UNP P24295
A	380	VAL	SER	engineered mutation	UNP P24295

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	40	Total 40	O 40	0	0

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: NAD-SPECIFIC GLUTAMATE DEHYDROGENASE
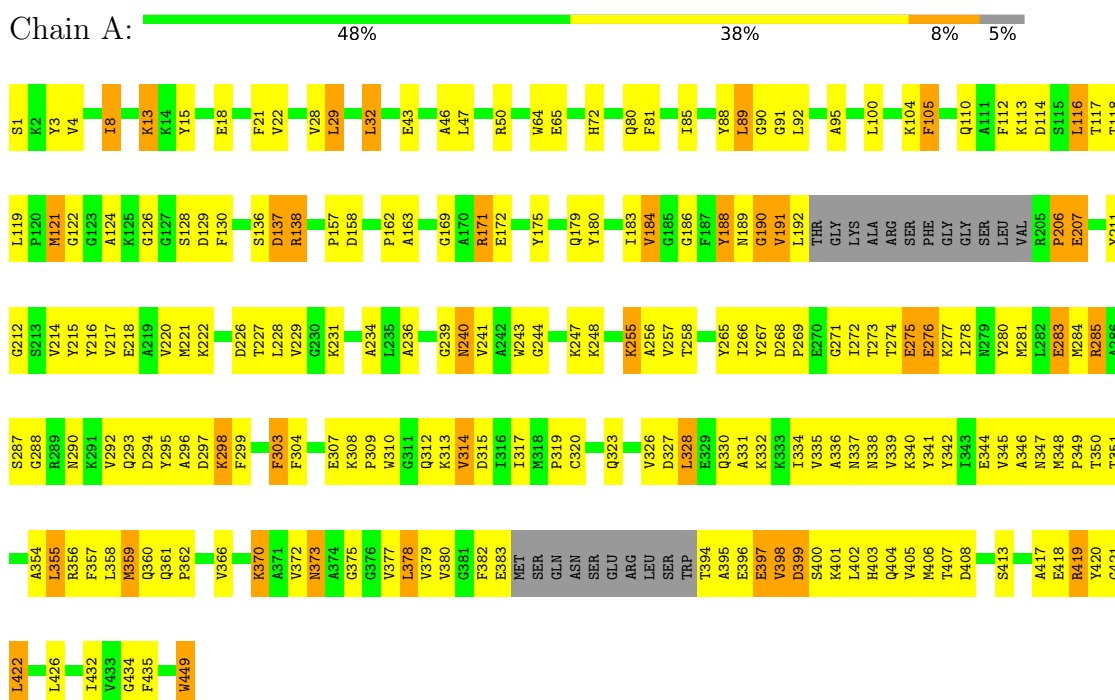
4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	162.90Å 162.90Å 100.70Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	18.00 – 2.50	Depositor
% Data completeness (in resolution range)	99.0 (18.00-2.50)	Depositor
R_{merge}	0.14	Depositor
R_{sym}	0.07	Depositor
Refinement program	TNT 5E	Depositor
R, R_{free}	0.190 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3315	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

5   Model quality (i)

5.1   Standard geometry (i)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$ >5	RMSZ	#$|Z|$ >5
1	A	0.69	0/3344	0.64	2/4524 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	207	GLU	N-CA-C	-6.40	93.71	111.00
1	A	397	GLU	N-CA-C	-5.24	96.85	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2   Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3275	0	3196	247	1
2	A	40	0	0	2	0
All	All	3315	0	3196	247	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 38.

All (247) 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:417:ALA:HA	1:A:422:LEU:HD12	1.27	1.15
1:A:310:TRP:HD1	1:A:330:GLN:HG2	1.10	1.15
1:A:310:TRP:CD1	1:A:330:GLN:HG2	1.84	1.12
1:A:335:VAL:HG11	1:A:361:GLN:HG3	1.35	1.08
1:A:29:LEU:HA	1:A:32:LEU:HD12	1.15	1.07
1:A:417:ALA:CA	1:A:422:LEU:HD12	1.83	1.07
1:A:241:VAL:HG13	1:A:320:CYS:HB3	1.37	1.06
1:A:335:VAL:CG1	1:A:361:GLN:HG3	1.87	1.04
1:A:119:LEU:HB2	1:A:121:MET:HE2	1.41	1.01
1:A:357:PHE:O	1:A:360:GLN:HB2	1.65	0.96
1:A:304:PHE:HB3	1:A:307:GLU:OE2	1.66	0.95
1:A:243:TRP:HB2	1:A:281:MET:HE2	1.47	0.94
1:A:215:TYR:HE1	1:A:248:LYS:HE3	1.32	0.93
1:A:417:ALA:HA	1:A:422:LEU:CD1	2.00	0.92
1:A:379:VAL:O	1:A:382:PHE:HB2	1.69	0.92
1:A:119:LEU:HD12	1:A:121:MET:CE	2.01	0.90
1:A:398:VAL:O	1:A:400:SER:N	2.03	0.90
1:A:310:TRP:HB2	1:A:330:GLN:HG3	1.56	0.88
1:A:281:MET:HA	1:A:284:MET:CE	2.03	0.88
1:A:29:LEU:HA	1:A:32:LEU:CD1	2.01	0.87
1:A:310:TRP:HD1	1:A:330:GLN:CG	1.87	0.87
1:A:310:TRP:CD1	1:A:330:GLN:CG	2.59	0.85
1:A:119:LEU:HD12	1:A:121:MET:HE1	1.56	0.85
1:A:314:VAL:O	1:A:339:VAL:HG13	1.77	0.84
1:A:47:LEU:O	1:A:47:LEU:HD12	1.78	0.84
1:A:394:THR:OG1	1:A:397:GLU:HG3	1.80	0.82
1:A:215:TYR:CE1	1:A:248:LYS:HE3	2.14	0.82
1:A:255:LYS:HG3	1:A:271:GLY:HA3	1.62	0.82
1:A:330:GLN:O	1:A:334:ILE:HG13	1.80	0.81
1:A:266:ILE:HG22	1:A:303:PHE:HB2	1.61	0.81
1:A:184:VAL:HG23	1:A:186:GLY:H	1.46	0.81
1:A:188:TYR:HD2	1:A:189:ASN:H	1.27	0.81
1:A:207:GLU:O	1:A:211:TYR:CG	2.34	0.81
1:A:310:TRP:HB2	1:A:330:GLN:HE21	1.47	0.79
1:A:298:LYS:HG3	1:A:299:PHE:CD2	2.17	0.78
1:A:255:LYS:HB2	1:A:273:THR:CG2	2.14	0.77
1:A:354:ALA:O	1:A:357:PHE:HB3	1.85	0.77
1:A:89:LEU:HD21	1:A:377:VAL:HG23	1.64	0.76
1:A:119:LEU:CB	1:A:121:MET:HE2	2.15	0.75
1:A:243:TRP:N	1:A:281:MET:HE1	2.01	0.75
1:A:335:VAL:HG11	1:A:361:GLN:CG	2.16	0.74
1:A:188:TYR:CD2	1:A:189:ASN:N	2.55	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:TRP:CB	1:A:330:GLN:HE21	2.00	0.73
1:A:241:VAL:CG1	1:A:320:CYS:HB3	2.15	0.73
1:A:215:TYR:CE1	1:A:248:LYS:CE	2.72	0.73
1:A:267:TYR:CE2	1:A:269:PRO:HG3	2.24	0.73
1:A:255:LYS:HB2	1:A:273:THR:HG23	1.71	0.72
1:A:310:TRP:HB2	1:A:330:GLN:CG	2.20	0.72
1:A:281:MET:HA	1:A:284:MET:HE2	1.69	0.72
1:A:310:TRP:HB2	1:A:330:GLN:NE2	2.06	0.71
1:A:212:GLY:HA3	1:A:406:MET:HE2	1.70	0.70
1:A:162:PRO:O	1:A:191:VAL:O	2.10	0.69
1:A:206:PRO:HB2	1:A:240:ASN:OD1	1.93	0.69
1:A:256:ALA:C	1:A:272:ILE:HD12	2.13	0.68
1:A:335:VAL:HG12	1:A:361:GLN:HG3	1.71	0.68
1:A:266:ILE:CG2	1:A:303:PHE:HB2	2.23	0.68
1:A:190:GLY:C	1:A:192:LEU:H	1.95	0.68
1:A:399:ASP:O	1:A:403:HIS:HB2	1.93	0.68
1:A:402:LEU:O	1:A:406:MET:HG2	1.94	0.68
1:A:398:VAL:O	1:A:399:ASP:C	2.32	0.67
1:A:310:TRP:CB	1:A:330:GLN:HG3	2.23	0.66
1:A:266:ILE:HG22	1:A:303:PHE:HA	1.78	0.66
1:A:357:PHE:O	1:A:360:GLN:CB	2.43	0.65
1:A:89:LEU:CD2	1:A:377:VAL:HG23	2.26	0.65
1:A:327:ASP:HA	1:A:351:THR:HG23	1.79	0.65
1:A:379:VAL:O	1:A:382:PHE:N	2.30	0.64
1:A:90:GLY:O	1:A:162:PRO:HA	1.97	0.64
1:A:207:GLU:HG3	1:A:243:TRP:CZ3	2.33	0.63
1:A:266:ILE:HG22	1:A:303:PHE:CB	2.28	0.63
1:A:331:ALA:O	1:A:335:VAL:HG22	1.97	0.63
1:A:358:LEU:O	1:A:361:GLN:N	2.32	0.63
1:A:350:THR:HG22	1:A:354:ALA:HB3	1.80	0.63
1:A:379:VAL:HA	1:A:382:PHE:CD2	2.34	0.63
1:A:323:GLN:HA	1:A:348:MET:O	1.99	0.63
1:A:169:GLY:N	1:A:172:GLU:OE1	2.29	0.63
1:A:47:LEU:HD12	1:A:47:LEU:C	2.18	0.63
1:A:217:VAL:CG1	1:A:228:LEU:HD21	2.28	0.62
1:A:29:LEU:HD22	1:A:32:LEU:CD1	2.30	0.62
1:A:373:ASN:HD22	1:A:373:ASN:C	2.04	0.61
1:A:217:VAL:HG11	1:A:228:LEU:HD21	1.81	0.61
1:A:265:TYR:CD2	1:A:309:PRO:HB3	2.36	0.60
1:A:4:VAL:O	1:A:8:ILE:HG13	2.01	0.60
1:A:239:GLY:HA2	1:A:285:ARG:HD2	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:LYS:HG3	1:A:271:GLY:CA	2.30	0.60
1:A:239:GLY:HA2	1:A:285:ARG:CD	2.32	0.60
1:A:449:TRP:CE3	1:A:449:TRP:HA	2.36	0.59
1:A:327:ASP:C	1:A:354:ALA:HB2	2.21	0.59
1:A:190:GLY:O	1:A:192:LEU:N	2.34	0.59
1:A:137:ASP:OD2	1:A:175:TYR:OH	2.10	0.59
1:A:231:LYS:HD2	1:A:315:ASP:HB3	1.84	0.59
1:A:346:ALA:O	1:A:349:PRO:HG3	2.03	0.59
1:A:417:ALA:CB	1:A:422:LEU:HD12	2.33	0.58
1:A:188:TYR:HD2	1:A:189:ASN:N	1.97	0.58
1:A:266:ILE:HG22	1:A:303:PHE:CA	2.33	0.58
1:A:293:GLN:O	1:A:296:ALA:N	2.36	0.58
1:A:281:MET:HA	1:A:284:MET:HE3	1.86	0.58
1:A:356:ARG:HA	1:A:359:MET:HG3	1.85	0.58
1:A:304:PHE:HB3	1:A:307:GLU:CD	2.23	0.58
1:A:119:LEU:HD12	1:A:121:MET:HE2	1.85	0.58
1:A:331:ALA:HB1	1:A:358:LEU:HD21	1.86	0.58
1:A:207:GLU:O	1:A:211:TYR:CB	2.51	0.57
1:A:226:ASP:OD1	1:A:227:THR:N	2.32	0.57
1:A:243:TRP:CB	1:A:281:MET:HE2	2.26	0.57
1:A:117:THR:C	1:A:118:THR:HG23	2.25	0.57
1:A:327:ASP:HA	1:A:351:THR:CG2	2.34	0.57
1:A:243:TRP:HZ2	1:A:247:LYS:NZ	2.02	0.57
1:A:255:LYS:HB2	1:A:273:THR:HG21	1.84	0.57
1:A:401:LYS:O	1:A:405:VAL:HG23	2.05	0.56
1:A:243:TRP:CZ2	1:A:247:LYS:NZ	2.73	0.56
1:A:29:LEU:HD22	1:A:32:LEU:HD12	1.86	0.56
1:A:243:TRP:CD1	1:A:278:ILE:HG23	2.40	0.56
1:A:215:TYR:CZ	1:A:248:LYS:HE2	2.40	0.56
1:A:350:THR:HG21	1:A:355:LEU:HD12	1.87	0.56
1:A:215:TYR:OH	1:A:248:LYS:HE2	2.05	0.56
1:A:379:VAL:O	1:A:382:PHE:CB	2.49	0.56
1:A:398:VAL:C	1:A:400:SER:N	2.58	0.56
1:A:243:TRP:HD1	1:A:278:ILE:HG23	1.71	0.55
1:A:396:GLU:C	1:A:398:VAL:N	2.56	0.55
1:A:243:TRP:HZ2	1:A:247:LYS:HZ3	1.53	0.55
1:A:274:THR:OG1	1:A:277:LYS:HD2	2.06	0.55
1:A:350:THR:CG2	1:A:354:ALA:HB3	2.36	0.55
1:A:215:TYR:OH	1:A:248:LYS:CE	2.55	0.55
1:A:236:ALA:HB2	1:A:310:TRP:CZ2	2.41	0.55
1:A:216:TYR:O	1:A:220:VAL:HG23	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:LYS:C	1:A:298:LYS:CD	2.75	0.54
1:A:116:LEU:CD1	1:A:434:GLY:CA	2.86	0.54
1:A:29:LEU:N	1:A:29:LEU:HD23	2.22	0.54
1:A:184:VAL:CG2	1:A:186:GLY:H	2.18	0.53
1:A:345:VAL:HG22	1:A:372:VAL:HG11	1.89	0.53
1:A:417:ALA:C	1:A:422:LEU:HD12	2.28	0.53
1:A:267:TYR:CZ	1:A:269:PRO:HG3	2.44	0.53
1:A:294:ASP:HA	1:A:297:ASP:OD2	2.08	0.53
1:A:21:PHE:CE2	1:A:104:LYS:HE2	2.44	0.53
1:A:207:GLU:O	1:A:211:TYR:HB2	2.08	0.53
1:A:347:ASN:O	1:A:348:MET:C	2.48	0.52
1:A:190:GLY:C	1:A:192:LEU:N	2.63	0.52
1:A:88:TYR:HB3	1:A:124:ALA:HB2	1.91	0.51
1:A:327:ASP:O	1:A:354:ALA:HB2	2.09	0.51
1:A:394:THR:O	1:A:398:VAL:HG23	2.10	0.51
1:A:284:MET:SD	1:A:295:TYR:HB2	2.51	0.51
1:A:117:THR:OG1	1:A:119:LEU:HG	2.11	0.51
1:A:211:TYR:N	1:A:211:TYR:CD1	2.77	0.51
1:A:257:VAL:HG23	1:A:258:THR:HG23	1.92	0.51
1:A:207:GLU:HG3	1:A:243:TRP:CH2	2.46	0.50
1:A:119:LEU:CG	1:A:121:MET:HE2	2.40	0.50
1:A:281:MET:CA	1:A:284:MET:CE	2.85	0.50
1:A:418:GLU:O	1:A:421:GLY:N	2.25	0.50
1:A:257:VAL:HA	1:A:268:ASP:O	2.12	0.50
1:A:116:LEU:HD11	1:A:434:GLY:N	2.26	0.50
1:A:211:TYR:HE1	1:A:244:GLY:O	1.95	0.50
1:A:298:LYS:C	1:A:298:LYS:HD3	2.32	0.50
1:A:236:ALA:HB2	1:A:310:TRP:CH2	2.46	0.49
1:A:28:VAL:HG12	1:A:32:LEU:HD11	1.95	0.49
1:A:215:TYR:CE1	1:A:248:LYS:HE2	2.45	0.49
1:A:281:MET:CA	1:A:284:MET:HE2	2.42	0.49
1:A:234:ALA:HA	1:A:258:THR:OG1	2.13	0.49
1:A:274:THR:O	1:A:276:GLU:N	2.45	0.49
1:A:89:LEU:CD2	1:A:377:VAL:CG2	2.91	0.49
1:A:64:TRP:CE2	1:A:72:HIS:HB2	2.48	0.49
1:A:117:THR:O	1:A:118:THR:HG23	2.13	0.48
1:A:283:GLU:O	1:A:287:SER:HB3	2.13	0.48
1:A:243:TRP:N	1:A:281:MET:CE	2.74	0.48
1:A:375:GLY:HA2	1:A:402:LEU:HD11	1.96	0.48
1:A:171:ARG:HD2	1:A:172:GLU:OE2	2.13	0.48
1:A:18:GLU:O	1:A:22:VAL:HG23	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:VAL:HG13	1:A:320:CYS:CB	2.26	0.48
1:A:366:VAL:O	1:A:426:LEU:HB2	2.14	0.48
1:A:317:ILE:HG22	1:A:319:PRO:HD3	1.95	0.48
1:A:317:ILE:HB	1:A:342:TYR:HD1	1.79	0.48
1:A:1:SER:HB3	1:A:4:VAL:HB	1.96	0.47
1:A:298:LYS:HG3	1:A:299:PHE:CG	2.49	0.47
1:A:317:ILE:HG21	1:A:342:TYR:CE1	2.49	0.47
1:A:180:TYR:CE1	1:A:184:VAL:HG21	2.50	0.47
1:A:274:THR:O	1:A:275:GLU:C	2.53	0.47
1:A:211:TYR:CE1	1:A:244:GLY:O	2.68	0.46
1:A:277:LYS:HA	1:A:299:PHE:CE2	2.50	0.46
1:A:394:THR:HB	1:A:395:ALA:H	1.42	0.46
1:A:419:ARG:HG2	1:A:420:TYR:CD2	2.50	0.46
1:A:243:TRP:CA	1:A:281:MET:CE	2.93	0.46
1:A:183:ILE:HG22	1:A:184:VAL:N	2.30	0.46
1:A:326:VAL:N	1:A:349:PRO:O	2.44	0.46
1:A:358:LEU:C	1:A:360:GLN:N	2.68	0.46
1:A:215:TYR:CZ	1:A:248:LYS:CE	2.97	0.46
1:A:340:LYS:HD3	1:A:341:TYR:CZ	2.50	0.46
1:A:28:VAL:O	1:A:32:LEU:HG	2.16	0.46
1:A:336:ALA:C	1:A:337:ASN:HD22	2.20	0.46
1:A:379:VAL:O	1:A:380:VAL:C	2.52	0.46
1:A:112:PHE:HE2	1:A:435:PHE:HB2	1.80	0.46
1:A:114:ASP:OD2	1:A:122:GLY:O	2.33	0.46
1:A:179:GLN:HA	1:A:179:GLN:OE1	2.14	0.46
1:A:358:LEU:O	1:A:359:MET:C	2.53	0.45
1:A:256:ALA:O	1:A:272:ILE:HD12	2.16	0.45
1:A:418:GLU:O	1:A:419:ARG:C	2.55	0.45
1:A:271:GLY:O	1:A:277:LYS:NZ	2.44	0.45
1:A:46:ALA:O	1:A:50:ARG:HG3	2.15	0.45
1:A:398:VAL:O	1:A:401:LYS:N	2.49	0.45
1:A:355:LEU:O	1:A:359:MET:HG2	2.16	0.45
1:A:15:TYR:HA	2:A:465:HOH:O	2.17	0.45
1:A:310:TRP:CB	1:A:330:GLN:CG	2.90	0.45
1:A:256:ALA:CB	1:A:272:ILE:HD12	2.48	0.44
1:A:80:GLN:HB3	1:A:88:TYR:CE2	2.53	0.44
1:A:128:SER:C	1:A:130:PHE:H	2.20	0.44
1:A:378:LEU:HD13	1:A:378:LEU:HA	1.90	0.44
1:A:304:PHE:CD1	1:A:304:PHE:N	2.85	0.44
1:A:346:ALA:O	1:A:349:PRO:CG	2.66	0.44
1:A:119:LEU:CD1	1:A:121:MET:HE2	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:ARG:HA	1:A:138:ARG:HD3	1.64	0.44
1:A:92:LEU:HA	1:A:126:GLY:O	2.18	0.44
1:A:100:LEU:O	1:A:104:LYS:HB2	2.18	0.44
1:A:350:THR:CG2	1:A:355:LEU:HD12	2.48	0.43
1:A:344:GLU:OE2	1:A:355:LEU:HD11	2.18	0.43
1:A:338:ASN:HB3	2:A:483:HOH:O	2.18	0.43
1:A:105:PHE:CD1	1:A:105:PHE:C	2.91	0.43
1:A:215:TYR:CD2	1:A:403:HIS:HA	2.53	0.43
1:A:212:GLY:C	1:A:406:MET:HE3	2.39	0.43
1:A:256:ALA:O	1:A:271:GLY:HA2	2.19	0.43
1:A:404:GLN:O	1:A:407:THR:HB	2.19	0.43
1:A:95:ALA:O	1:A:129:ASP:HA	2.18	0.43
1:A:211:TYR:N	1:A:211:TYR:HD1	2.17	0.43
1:A:276:GLU:H	1:A:276:GLU:HG3	1.59	0.42
1:A:405:VAL:HA	1:A:408:ASP:OD2	2.19	0.42
1:A:296:ALA:HB2	1:A:303:PHE:HB2	2.01	0.42
1:A:417:ALA:O	1:A:422:LEU:HD12	2.19	0.42
1:A:214:VAL:HG21	1:A:248:LYS:HB3	2.01	0.42
1:A:308:LYS:HB3	1:A:330:GLN:NE2	2.34	0.42
1:A:217:VAL:O	1:A:220:VAL:HB	2.20	0.42
1:A:280:TYR:O	1:A:284:MET:HE2	2.20	0.42
1:A:91:GLY:HA2	1:A:163:ALA:H	1.84	0.42
1:A:231:LYS:HD2	1:A:315:ASP:CB	2.50	0.42
1:A:3:TYR:CD1	1:A:43:GLU:HG3	2.55	0.42
1:A:21:PHE:CD2	1:A:104:LYS:HE2	2.54	0.42
1:A:370:LYS:HB3	1:A:370:LYS:HE3	1.88	0.42
1:A:85:ILE:HD11	1:A:121:MET:O	2.20	0.41
1:A:327:ASP:O	1:A:354:ALA:CB	2.68	0.41
1:A:110:GLN:O	1:A:110:GLN:HG3	2.19	0.41
1:A:218:GLU:OE1	1:A:403:HIS:NE2	2.48	0.41
1:A:407:THR:HG22	1:A:408:ASP:N	2.35	0.41
1:A:113:LYS:NZ	1:A:373:ASN:HD21	2.19	0.41
1:A:361:GLN:HA	1:A:362:PRO:HD3	1.71	0.41
1:A:293:GLN:O	1:A:297:ASP:N	2.49	0.40
1:A:212:GLY:CA	1:A:406:MET:HE2	2.48	0.40
1:A:215:TYR:OH	1:A:248:LYS:NZ	2.53	0.40
1:A:328:LEU:HD22	1:A:332:LYS:HE3	2.04	0.40
1:A:373:ASN:C	1:A:373:ASN:ND2	2.72	0.40
1:A:348:MET:N	1:A:349:PRO:HD3	2.36	0.40
1:A:355:LEU:O	1:A:356:ARG:C	2.59	0.40
1:A:290:ASN:HD22	1:A:290:ASN:HA	1.67	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:LYS:NZ	1:A:312:GLN:OE1[14_554]	2.11	0.09

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	421/449 (94%)	367 (87%)	44 (10%)	10 (2%)	6 9

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	188	TYR
1	A	191	VAL
1	A	206	PRO
1	A	399	ASP
1	A	398	VAL
1	A	275	GLU
1	A	190	GLY
1	A	157	PRO
1	A	229	VAL
1	A	288	GLY

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	337/358 (94%)	297 (88%)	40 (12%)	5 10

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ILE
1	A	13	LYS
1	A	29	LEU
1	A	32	LEU
1	A	65	GLU
1	A	81	PHE
1	A	89	LEU
1	A	105	PHE
1	A	116	LEU
1	A	121	MET
1	A	136	SER
1	A	137	ASP
1	A	138	ARG
1	A	158	ASP
1	A	171	ARG
1	A	184	VAL
1	A	221	MET
1	A	222	LYS
1	A	240	ASN
1	A	255	LYS
1	A	276	GLU
1	A	283	GLU
1	A	285	ARG
1	A	292	VAL
1	A	298	LYS
1	A	303	PHE
1	A	313	LYS
1	A	314	VAL
1	A	328	LEU
1	A	355	LEU
1	A	359	MET
1	A	370	LYS
1	A	373	ASN
1	A	378	LEU
1	A	383	GLU
1	A	413	SER
1	A	419	ARG
1	A	422	LEU

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Mol	Chain	Res	Type
1	A	432	ILE
1	A	449	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	290	ASN
1	A	324	ASN
1	A	330	GLN
1	A	337	ASN
1	A	360	GLN
1	A	373	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.