Appendix 1

Feature Importance

Feature_name	importance
lbp_3D_k_gldm_DependenceVariance_h1	0.18
logarithm_glszm_SizeZoneNonUniformityNormalized_h1	0.17
lbp_3D_k_glcm_SumSquares_h1	0.12
lbp_3D_k_glcm_InverseVariance_h1	0.11
logarithm_glszm_GrayLevelNonUniformityNormalized_h1	0.11
exponential_glrlm_ShortRunLowGrayLevelEmphasis_h2	0.09
squareroot_glszm_GrayLevelVariance_h2	0.09
gradient_glszm_SmallAreaEmphasis_h2	0.06
log_sigma_2_0_mm_3D_glszm_SmallAreaHighGrayLevelEmphasis_h3	0.04
logarithm_gldm_SmallDependenceHighGrayLevelEmphasis_h3	0.03

Study Population

We used data from a published double-blind, randomised, phase III clinical trial (ClinicalTrials.gov: NCT03607539), which was conducted between 23 August 2018 and 15 November 2019 conducted between 26 July 2018 and 7 July 2019 with baseline CT scans. The validation cohort enrolled from Institution I and from Institution II. Inclusion criteria were (I) availability of TPS data from target tumour biopsies, (II) availability of baseline contrast-enhanced arterial-phase CT images, (III) target tumour images were clear and free of artefacts, and (IV) receipt of anti-PD1 combination therapy. Exclusion criteria were (I) baseline contrast-enhanced arterial-phase CT images were corrupted or unavailable; (II) target tumour could not be clearly identified or was interfered by artefacts; and (III) clinical information was incomplete. *Table 1* illustrates the clinical characteristics of the patients and *Figure 1* shows the patient screening process.

Imaging Acquisition and Preprocessing

Tumour Cell Proportion Score (TPS)

Tumour cell proportion score (TPS) data were obtained from publicly available clinical trial data (ClinicalTrials.gov: NCT03607539). PD-L1 expression in tumour specimens was assayed by using the PD-L1 IHC 22C3 pharmDx kit (Agilent Technologies, Beijing, China) at the Kovensky Core Laboratory in Shanghai. The kit calculates the percentage of surviving tumour cells with partial or complete membrane staining to obtain a TPS for measuring PD-L1 expression in tumour biopsy specimens.

In the internal validation cohort, the model achieved an AUC of 0.911 (95% CI: 0.861–0.961), while in the external validation cohort, the AUC was 0.758 (95% CI: 0.675–0.842) (*Figure S2*). Performance metrics in the external validation cohort included a sensitivity of 0.673, specificity of 0.733, PPV of 0.600, and NPV of 0.781. Confusion matrices (CM) for the training cohort and validation cohort (F). A balanced distribution between the training and validation cohorts suggests good generalizability of the model.

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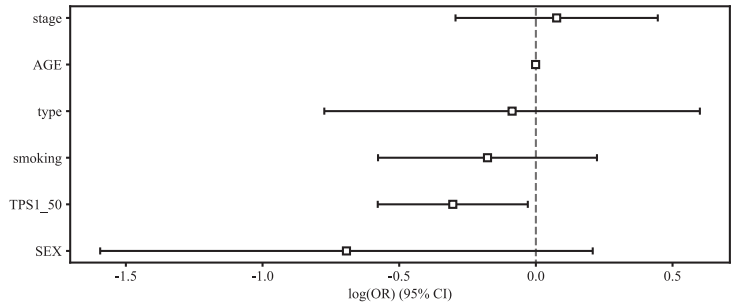

Figure S1 Extended logistic regression analysis. Figure presents an extended logistic regression analysis examining the impact of various clinical characteristics on disease progression prediction. The final model included stage, age, disease type, smoking history, tumor proportion score (TPS1_50), and sex as predictive variables. Age was evaluated as a continuous variable, while the other factors were analyzed as categorical variables. The results indicated that TPS1_50 (OR = -0.304) was significantly associated with disease progression, suggesting its potential role in influencing disease outcomes.

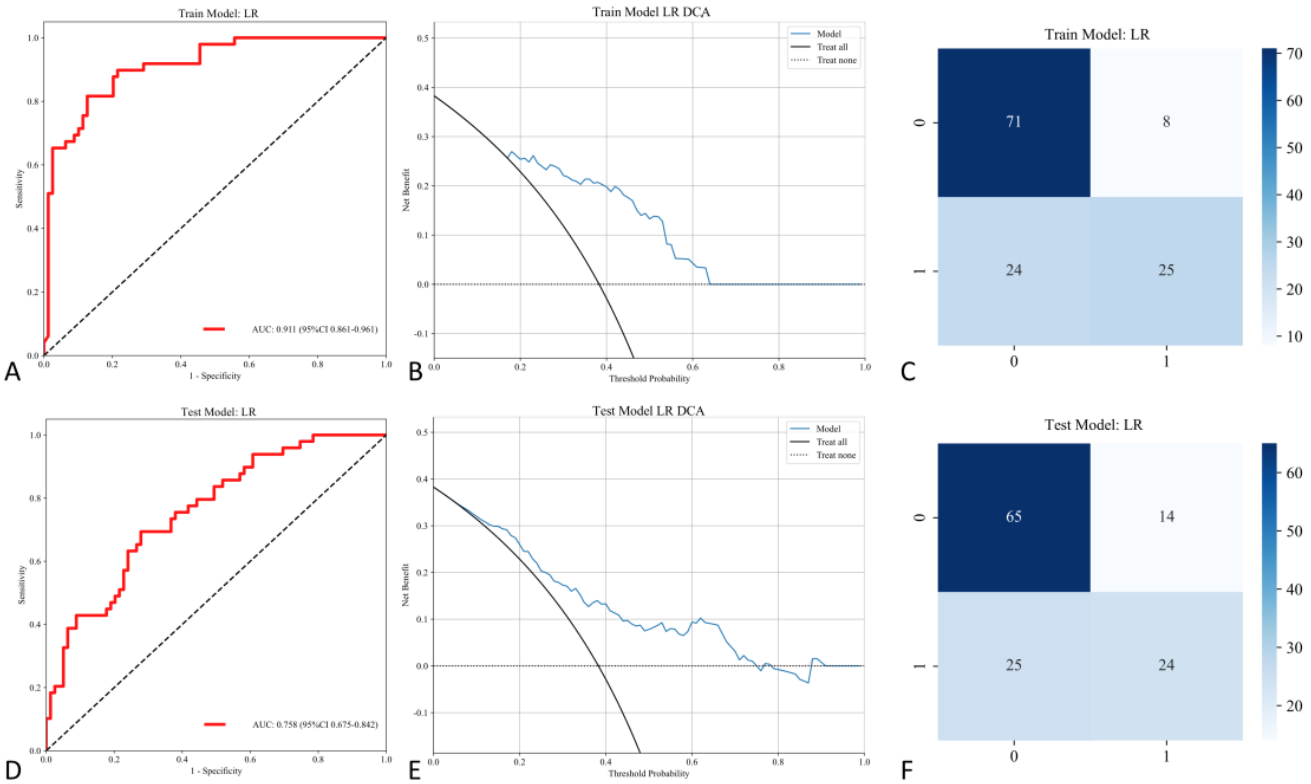

Figure S2 Performance evaluation of the predictive model in the training and validation cohorts. (A) Receiver Operating Characteristic (ROC) curves for the training cohort and validation cohort (D). (B) Decision Curve Analysis (DCA) curves for the training cohort and validation cohort (E). (C) Confusion matrices (CM) for the training cohort and validation cohort (F).

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